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! ***** !
! ** Mechanism for the pyrolysis and oxidation of anisole ** !
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! ** NOWAKOWSKA, HERBINET, DUFOUR, GLAUDE ** !
! ** LRGP 2013 ** !
! ** ** !
! ** ** !
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! ***** !

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ELEMENTS
H O C N AR HE
END

SPECIES

!*****!

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AR
N2
HE
B2CO
H2
H2O
O2
CH4
CO2
C2H2      !ch//ch          acetylene
C2H4Z     !ch2//ch2         ethylene
C2H6      !ch3/ch3          ethane
aC3H4     !ch2//ch//ch2    propadiene = allene
pC3H4     !ch//c/ch3        propyne
C3H6Y     !ch2//ch/ch3      propylene = propene
C3H8      !ch3/ch2/ch3    propane
C4H2      !ch//c/c//ch    butadiyne = diacetylene
C4H4      !ch2//ch/c//ch   1-buten-3-yne ou vinyl
acetylene
C4H6Z2    !ch2//ch/ch//ch2  butadiene
C4H6-12   !ch2//c//ch/ch3    1,2-butadiène ou
méthyl allène
C4H6-1    !ch//c/ch2/ch3      1-butyne
C4H6-2    !ch3/c//c/ch3       2-butyne
C4H8Y     !ch2//ch/ch2/ch3    butene
iC4H8     !ch2//c(ch3)/ch3    2methyl-propene
C4H10     !ch3/ch2/ch2/ch3    butane
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

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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

! ajout anisole

anisole !C6H5#/O/CH3
 C6H5#OCH2 ! rad anisole
 !C6H5CH2O rad from C6H5#OCH2

! Biradicals :

B1O
 B3C
 B4CH
 B5CH2
 B6CH2
 C3H2 !.ch//c//c(.)h

! Primary molecules :

H2O2
 HCHO
 CH3OH
 CH3OOH
 C2H4O#3 !c(#1)h2/o/ch2/1
 CH2COZ !ch2//c//o
 CH3CHO !ch(/o)/ch3
 !CH3OCH3 !MF car n'intervient plus (une réaction)
 !CH3OOCH3 !MF car n'intervient plus (une réaction)
 C3H7OH
 C2H6CO
 C3H8CO !C4H8OK = butanone
 C2H5CHO !ch(/o)/ch2/ch3 propanal
 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 réaction)
 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
 CH3COOOH !peracetic acid
 C2H5OOH !ethyl hydroperoxide
 C2H5OH !ethanol

!Espèces excitées

OHE

CHE

! 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	!acetylperoxy radical
R19C3H7	!.ch2/ch2/ch3	
R20C4H9		
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 réaction)
C6H4#	!.c(#1)&ch&ch&ch&ch&c(.)&1	
C6H5#	!.c(#1)&ch&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
aC3H3 !CH2=C=CH*

! MECHANISM OF BENZENE

! Molecules

C4H4O !ch2//ch/ch//c//o vinylketene
!C5H6 !ch//c/ch//ch/ch3 !MF car n'intervient plus (une
réaction)
C5H5OH# !c(#1)h//ch/ch//ch/ch(/oh)/1 cyclopentadienol
C6H5OH# !c(#1)h&ch&ch&ch&ch&c(/oh)&1 phénol
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 réaction)
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&ch&c&2)&1
C6H5OOH

C6H5C3H3
fulvene

! Radicals

C5H5# !c(#1)(.)h/ch//ch/ch//ch/1
!C5H5 !.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&c(/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
HOC6H4CH2OO !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

!*Especes 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#OOH !C6H5#ch(/ooh)/ch3 !c(#1)h&ch&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1
 C8H9#O !C6H5#ch(/o.)/ch3 !c(#1)h&ch&ch&ch&ch&c(/ch(/o.)/ch3)&1
 OOC6H4CH3 !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
 TolOCH2C6H5 !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
 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
 bicycle
 (H)(CH3)C6H4O
 guaiacol
 HOC6H5#C2H5 !ch(#1)&ch&ch&ch&c(/oh)&c(/ch2/ch3)&1
 HOC6H5#C2H4 !ch(#1)&ch&ch&ch&c(/oh)&c(/ch./ch3)&1
 HOstyrene !ch(#1)&ch&ch&ch&c(/oh)&c(ch//ch2)&1

! MECHANISM OF INDANE (molecules)

indane
 ph#C3H5Z !c(#1)&ch&ch&ch&ch&ch&1,1//ch2/ch//ch2
 ph#C3H5p !c(#1)&ch&ch&ch&ch&ch&1,1/ch//ch/ch3
 ph#C3H7 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/ch2/ch3
 ph#C4H9 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/ch2/ch2/ch3
 C2H3C6H4CHO
 !CH3C6H4C3H7 !c(#1)(/ch2/ch2/ch3)&c(/ch3)&ch&ch&ch&ch&1
 C9H8O# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/c(/o)/ch2/ch2/2
 methylindane !c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch3)/ch2/ch2/2
 !C2H3C6H4C2H5 !c(#1)(/ch2/ch3)&c(/ch//ch2)&ch&ch&ch&ch&1
 !C2H3C6H4CH2OH !c(#1)(/ch//ch2)&c(/ch2/oh)&ch&ch&ch&ch&1
 C9H6O# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/c(/o)/ch//ch/2
 !ph#C4H5 !c(#1)&ch&ch&ch&ch&ch&1,1/ch(/ch3)/c//ch
 C3H5C6H4CH3 !c(#1)&c(#2)(/ch3)&ch&ch&ch&ch&1,1/c(/ch2)/ch3
 methylindene-2 !c(#1)&c(#2)&ch&ch&ch&ch&1,1/c(/ch3)//ch/ch2/2
 !ph#C4H7-2 !c(#1)&ch&ch&ch&ch&ch&1,1/CH2/CH//CH/CH3
 ph#C4H7-3 !c(#1)&ch&ch&ch&ch&ch&1,1/CH//CH/CH2/CH3

! MECHANISM OF INDANE (free radicals)

indanyl-Y !c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/)/ch2/ch2/2
 indanyl-1 !c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch2/ch(/)/ch2/2
 C3H5C6H4 !c(#1)(/ch2/ch//ch2)&c(/)/ch&ch&ch&ch&1
 CH3C6H4C3H6 !c(#1)(/ch2/ch2/ch2(/))&c(/ch3)&ch&ch&ch&ch&1
 C9H9O# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/o(/))/ch2/ch2/2
 C2H3C6H4CH2O !c(#1)(/ch//ch2)&c(/ch2/o(/))&ch&ch&ch&ch&1
 C3H5C6H4O !c(#1)(/ch2/ch//ch2)&c(/o(/))&ch&ch&ch&ch&1
 C9H7O# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/o(/))ch//ch/2
 !ph#C3H2 !c(#1)&ch&ch&ch&ch&ch&1,1/ch(/)/c//ch
 ph#C3H6-1 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/ch2/ch2(/)
 ph#C3H6-2 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/ch(/)/ch3
 ph#C3H6-Y !c(#1)&ch&ch&ch&ch&ch&1,1/ch(/)/ch2/ch3
 ph#C3H4Y !c(#1)&ch&ch&ch&ch&ch&1,1/ch(/)/ch//ch2
 ph#C3H4-1 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/ch//ch(/)
 ph#C3H4-2 !c(#1)&ch&ch&ch&ch&ch&1,1/ch2/c(/)//ch2
 ph#C3H4-3 !c(#1)&ch&ch&ch&ch&ch&1,1/c(/)//ch/ch3

ph#C3H4-4 ! c(#1)&ch&ch&ch&ch&ch&1,1/ch//c(./ch3
C10H11 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch3)/ch2/ch(./2
C10H11-1 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch3)/ch(./ch2/2
C10H11-2 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch2(./)/ch2/ch2/2
C10H11-3 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/c(./ch3)/ch2/ch2/2
!ph#C4H8-2 ! C6H5#/CH2/CH2/CH(./)CH3
!ph#C4H8-3 ! c(#1)&ch&ch&ch&ch&ch&1,1/CH2/CH./CH2/CH3
ph#C4H8X ! C6H5#/CH(./)CH2/CH2/CH3
C3H5C6H4CH2 ! c(#1)&c(#2)(/ch2(./)&ch&ch&ch&ch&1,1/c(/ch2)/ch3

A2C2H
A2CH3
A2CH2
phenanthrene
pyrene
CH3phenanth
CH2phenanth
A2R5
!chrysene
!C8H2
naphtol
A2O
C5H4CCH2
C5H5CCH
chrysene
antra
nC3H7
o-methylbenzyl
!C5H6
methylindene
S0 !9.10-dihydrofulvalene

!MECHANISM OF o-xylene

o-xylene
phenyl(CH3)2
HOC6H3(CH3)2
!.C3H5Y
OC6H3(CH3)2
CH3C6H4CHO
CH3C6H4CO
o-C6H4CHO
!C6H4CHO
CH3C6H4CH2OOH
CH3C6H4CH2O
CH3HOC6H3CH2
!o-OC6H4CHO
!C6H5CHO-1
CH3HOC6H3CH2OO
CH3HOC6H3CH2O
CH3C6H4OH#
CH3OHC6H3CHO
CH3C6H3OHCO

CH3C6H4CH2OH
CH3C6H4CHOH
CH3C6H4CH2CH3
CH3C6H4CHCH3
CH3styrene
o-bibenzyl
o-C14H13#
o-stilbene
benzocyclobut
benzocyclobutyl
styryl
!C2H2T
!C10H10
!C10H9
p-xylene
p-methylbenzyl
C6H5CHp-2
p-etC6H4
trimetbenz
p-xylylene
p-phtaldehyde
benzylCH2OH
HObenzylCH2OH
EnD

THERMO ALL

300.000 1000.000 5000.000

!especes excitees!

OHE C 0H 10 1 G 0300.00 5000.00 1000.00 1
3.04144E+00 6.51385E-04 -1.91218E-08 -1.04196E-13 4.00330E-17 2
5.17400E+04 4.81762E+00 3.67780E+00 -2.14153E-04 5.70231E-08 3
1.71404E-10 -1.84629E-14 5.17400E+04 1.19670E+00 4
CHE C 1H 1 G 0300.00 5000.00 1000.00 1
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
0.10500000E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04 3
0.05733890E-07-0.01955533E-10 0.10500000E+06 0.03331588E+02 4

!*Especes ajoutées*!

C6H5OOH mf-burcat T03/06C 6.H 6.0 2. 0.G 200.000 6000.000 1000. 1
1.61396041E+01 2.08447848E-02-7.64070773E-06 1.24667046E-09-7.51132000E-14 2
-7.68952573E+03-5.95754960E+01 2.63159057E-01 4.23800271E-02 3.05412431E-05 3
-8.13196326E-08 3.86504418E-11-2.41155401E+03 2.73095957E+01-3.22058666E+02 4
C5H4CCH2 cbd-qb3 pag C 7H 6 0 0G 300.000 5000.000 1396.000 1
1.68121948E+01 1.68679712E-02-5.85620989E-06 9.18454953E-10-5.36680000E-14 2
3.60029314E+04-6.67439600E+01-3.88857913E+00 7.16285896E-02-6.27290636E-05 3
2.81593703E-08-5.06188863E-12 4.25632251E+04 4.21812285E+01 4
C5H5CCH cbd-qb3 pag C 7H 6 0 0G 300.000 5000.000 1397.000 1
1.68972508E+01 1.67331982E-02-5.79543147E-06 9.07443659E-10-5.29640367E-14 2
4.09232497E+04-6.70082451E+01-3.90528821E+00 7.27894554E-02-6.51288475E-05 3
2.98127578E-08-5.44054969E-12 4.74164546E+04 4.20935797E+01 4
C5H5C2H2 QB3-MF-11 C 7H 70 0 G 0300.00 5000.00 1000.00 1

1.41364054E+01 2.38239499E-02-9.28122955E-06 1.65804186E-09-1.11439321E-13 2
5.14158755E+04-4.92894686E+01-5.87696103E+00 8.55461929E-02-7.96174009E-05 3
3.51343250E-08-5.01001292E-12 5.66076790E+04 5.24499022E+01 4
C6H5COCH3 MF THERGAS C 8H 80 1 G 0300.00 5000.00 1000.00 1
0.17828882E+02 0.27116600E-01-0.95296928E-05 0.15572350E-08-0.97619056E-13 2
-0.21163535E+05-0.68653084E+02-0.18458074E+01 0.75013384E-01-0.46304511E-04 3
0.88066798E-08 0.11858624E-11-0.15248022E+05 0.35008129E+02 4
C8H9#OOH MF THERGAS C 8H 100 2 G 0300.00 5000.00 1000.00 1
-0.31565318E+01 0.72488472E-01-0.31781656E-04 0.60659939E-08-0.42418182E-12 2
-0.75729609E+04 0.52722046E+02-0.80470219E+01 0.11141342E+00-0.84831234E-04 3
0.23181402E-07 0.13341983E-11-0.90922773E+04 0.67959465E+02 4
C8H9#O MF THERGAS C 8H 90 1 G 0300.00 5000.00 1000.00 1
-0.26841152E+01 0.63683085E-01-0.26554239E-04 0.48910964E-08-0.33337355E-12 2
0.11209342E+05 0.45193958E+02-0.10515040E+02 0.10946906E+00-0.87473454E-04 3
0.28099876E-07-0.67344112E-12 0.10719505E+05 0.76310471E+02 4
C6H5OCH2C6H5 MF THERGAS C 13H 120 1 G 0300.00 5000.00 1000.00 1
-0.63886577E+00 0.89705884E-01-0.38932521E-04 0.73697382E-08-0.51188193E-12 2
0.89398828E+03 0.37745117E+02-0.13924475E+02 0.14704998E+00-0.10288922E-03 3
0.23434016E-07 0.31243096E-11 0.20831367E+04 0.97889290E+02 4
ToIOCH2C6H5 MF THERGAS C 14H 140 1 G 0300.00 5000.00 1000.00 1
0.73168926E+01 0.84610440E-01-0.34892913E-04 0.63693735E-08-0.43093716E-12 2
-0.61409961E+04-0.40394058E+01-0.13099327E+02 0.15216646E+00-0.98755765E-04 3
0.17854818E-07 0.46560819E-11-0.21039302E+04 0.96266014E+02 4
PhenolCH2bz MF THERGAS C 13H 120 1 G 0300.00 5000.00 1000.00 1
0.53753876E+02 0.18723633E-02-0.61383815E-07-0.23911903E-11 0.33685039E-15 2
-0.25817414E+05-0.26792435E+03-0.65297952E+01 0.11671037E+00-0.62773179E-04 3
0.69906072E-08 0.11599543E-11-0.40289893E+04 0.62397514E+02 4
PhenolC2H4bz MF THERGAS C 14H 140 1 G 0300.00 5000.00 1000.00 1
0.59948162E+02 0.26446667E-02-0.13923673E-06 0.49298747E-11-0.12657805E-15 2
-0.31173285E+05-0.29929779E+03-0.44142666E+01 0.12597758E+00-0.69533759E-04 3
0.10197517E-07 0.23010318E-12-0.79399980E+04 0.53211372E+02 4
CH3bzOHCH2bz MF THERGAS C 14H 150 1 G 0300.00 5000.00 1000.00 1
0.80085793E+01 0.81080563E-01-0.32634987E-04 0.58541256E-08-0.39108004E-12 2
-0.10935330E+05-0.76485977E+01-0.99764366E+01 0.14664446E+00-0.10324772E-03 3
0.27777155E-07 0.59959589E-12-0.78735742E+04 0.78774628E+02 4
Benzaldtol MF THERGAS C 14H 120 2 G 0300.00 5000.00 1000.00 1
0.23387709E+02 0.53010050E-01-0.19097548E-04 0.31647776E-08-0.19974926E-12 2
-0.33023887E+05-0.90250610E+02-0.99071035E+01 0.13826986E+00-0.85146399E-04 3
0.12299934E-07 0.46802280E-11-0.23602482E+05 0.83241371E+02 4
HOC6H4CHO MF THERGAS C 7H 60 2 G 0300.00 5000.00 1000.00 1
0.26187965E+02 0.12539596E-01-0.39235060E-05 0.59002020E-09-0.34898333E-13 2
-0.37664734E+05-0.11374477E+03-0.24476035E+01 0.74593887E-01-0.45657820E-04 3
0.78774445E-08 0.98480870E-12-0.28170668E+05 0.40191536E+02 4
C6H5C4H7 MF THERGAS C 10H 120 0 G 0300.00 5000.00 1000.00 1
0.21914558E+02 0.33905298E-01-0.11222520E-04 0.17528664E-08-0.10622979E-12 2
0.29861094E+04-0.88769554E+02-0.40086384E+01 0.94950438E-01-0.55835400E-04 3
0.91944425E-08 0.19153808E-11 0.10992979E+05 0.48576912E+02 4
naphthalene MF BURCAT C 10H 8 0 OG 200.000 6000.000 1000. 1
1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13 2
8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05 3
-1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 1.81107678E+04 4
A2C2H OC 12H 80 0 G 0200.00 6000.00 1 !Slavinskaya09

2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13 2
3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05 3
-5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4.55914299E+04 4
A2CH3 OC 11H 100 0 G 0200.00 6000.00 1 !Slavinskaya09
2.17939213E+01 3.60214098E-02-1.33228698E-05 2.19304403E-09-1.33071380E-13 2
3.16261439E+03-9.48675403E+01-1.03043715E+00 6.03358177E-02 5.45655719E-05 3
-1.22769251E-07 5.54507327E-11 1.13241014E+04 3.22970611E+01 1.39642625E+04 4
A2CH2 OC 11H 90 0 G 0200.00 6000.00 1 !Slavinskaya09
2.18977539E+01 3.26102636E-02-1.18401218E-05 1.92574628E-09-1.15903442E-13 2
2.24571098E+04-9.41050741E+01-2.53234304E+00 7.32920338E-02 2.02974707E-05 3
-9.36547823E-08 4.70753594E-11 3.02906705E+04 3.79638513E+01 3.28097266E+04 4
phenanthrene OC 14H 100 0 G 0200.00 6000.00 1 !Slavinskaya09
0.26602474E+02 0.39769744E-01-0.14572026E-04 0.23843296E-08-0.14409548E-12 2
0.12132838E+05-0.12266672E+03-0.33646717E+01 0.85073271E-01 0.37531110E-04 3
-0.12664499E-06 0.61445705E-10 0.22019878E+05 0.40596218E+02 0.24908263E+05 4
A2R5 OC 12H 80 0 G 0300.00 5000.00 1 !Slavinskaya09,Burcat 2007
1.93183637E+01 3.90205238E-02-1.63352587E-05 3.10041991E-09-2.19199281E-13 2
2.15445149E+04-8.32372261E+01-2.81264181E+00 7.04681002E-02 3.15341955E-05 3
-1.05176189E-07 5.08713845E-11 2.88462829E+04 3.75755975E+01 3.12345526E+04 4
indenyl OC 9H 70 0 G 300.000 5000.000 1000. 1
1.59706473E+01 2.86651352E-02-1.12949950E-05 2.03414690E-09-1.37519923E-13 2
2.48192174E+04-6.29027317E+01-8.19315997E+00 9.69513671E-02-7.78644905E-05 3
2.41142048E-08 1.64713468E-13 3.14272288E+04 6.15513565E+01 4
naphthyl OC 10H 70 0 G 200.000 6000.000 1000. 1 !Base burcat!
1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14 2
3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
-9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4
C8H7O#-1 THERGAS OC 8H 70 1 G 0300.00 5000.00 1000.00 1
0.36577377E+01 0.48040181E-01-0.19457286E-04 0.35114045E-08-0.23589068E-12 2
0.52084609E+04-0.30909843E+01-0.60815744E+01 0.89198485E-01-0.67060450E-04 3
0.19099829E-07 0.30027036E-12 0.62320034E+04 0.41498894E+02 4
benzofuran BURCAT OC 8H 60 1 G 200.000 6000.00 1000.00 1
1.61267559E+01 2.42942790E-02-8.82919089E-06 1.43722155E-09-8.65592465E-14 2
-5.74867958E+03-6.40564836E+01-7.85221476E-01 3.96432449E-02 5.69751746E-05 3
-1.14831806E-07 5.19411145E-11 2.15748538E+02 3.02655928E+01 4
C8H8O# FOURNET OC 8H 80 1 G 0300.00 5000.00 1000.00 1
1.50839842E+01 3.25092066E-02-1.28403261E-05 2.31578474E-09-1.56702946E-13 2
-1.33912799E+04-5.85151857E+01-5.96220908E+00 8.15010579E-02-3.93920844E-05 3
-1.07682941E-08 1.14611472E-11-7.06811930E+03 5.25774976E+01 4
C8H7O# THERGAS OC 8H 70 1 G 0300.00 5000.00 1000.00 1
0.39498155E+01 0.47736809E-01-0.19333373E-04 0.34884815E-08-0.23430105E-12 2
0.10867305E+05-0.46506844E+01-0.64320035E+01 0.91989711E-01-0.72167728E-04 3
0.22816783E-07-0.66101562E-12 0.11987392E+05 0.42892570E+02 4
indene OC 9H 80 0 G 300.000 5000.000 1000.00 1
1.53776039E+01 3.21363915E-02-1.26700376E-05 2.28233298E-09-1.54312315E-13 2
1.08872191E+04-6.10238903E+01-7.49357917E+00 9.07281156E-02-5.76486055E-05 3
4.69816415E-09 6.61632944E-12 1.74727480E+04 5.83347582E+01 4
OOC6H4CH3 FAUX OC 7H 70 2 G 0300.00 5000.00 1000.00 1 !attention thermo fausse
1.53776039E+01 3.21363915E-02-1.26700376E-05 2.28233298E-09-1.54312315E-13 2
1.08872191E+04-6.10238903E+01-7.49357917E+00 9.07281156E-02-5.76486055E-05 3
4.69816415E-09 6.61632944E-12 1.74727480E+04 5.83347582E+01 4
cumene OC 9H 120 0 G 0300.00 5000.00 1000.00 1

0.16221073E+02 0.39657544E-01-0.14122924E-04 0.23296629E-08-0.14701162E-12 2
 -0.77848418E+04-0.61098145E+02-0.52103133E+01 0.95287584E-01-0.59495935E-04 3
 0.11685747E-07 0.16412634E-11-0.17408159E+04 0.50435326E+02 4
 C9H11#-1 OC 9H 11O OG 0300.00 5000.00 1000.00 1
 0.18773472E+02 0.32017492E-01-0.10167760E-04 0.15489963E-08-0.92642365E-13 2
 0.15833068E+05-0.71929497E+02-0.61953192E+01 0.10511646E+00-0.89499430E-04 3
 0.40374015E-07-0.77179487E-11 0.22515070E+05 0.56080315E+02 4
 CH3styre OC 9H 10O OG 0300.00 5000.00 1000.00 1!KINGAS
 -0.64905424E+01 0.74284628E-01-0.32960350E-04 0.63375678E-08-0.44518054E-12 2
 0.15234238E+05 0.65877571E+02-0.45196443E+01 0.92458449E-01-0.64155669E-04 3
 0.13829308E-07 0.29229772E-11 0.12028299E+05 0.46347641E+02 4
 C2H3C6H4CH2 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1
 1.70648122E+01 3.28892095E-02-1.28323249E-05 2.29479720E-09-1.54348164E-13 2
 2.48599234E+04-6.61223497E+01-5.67362805E+00 9.67482623E-02-7.49811328E-05 3
 2.31114824E-08-1.30018265E-14 3.11297550E+04 5.11628285E+01 4
 C6H5CH2CHO roda OC 8H 8O 1 G 0300.00 5000.00 1000.00 1
 0.36780437E+02-0.43310081E-02 0.48277348E-05-0.12297610E-08 0.10114482E-12 2
 -0.21796547E+05-0.17331140E+03 0.40768035E-01 0.61660051E-01-0.23909257E-04 3
 -0.23290552E-08 0.82279073E-12-0.83429141E+04 0.29040709E+02 4
 C6H5CH2CO C 8H 7O 1G 0300.00 5000.00 1000.00 1
 0.83566151E+01 0.37099533E-01-0.13471239E-04 0.22472100E-08-0.14262159E-12 2
 0.74995391E+04-0.11978180E+02-0.41511149E+01 0.78861803E-01-0.59583464E-04 3
 0.21248246E-07-0.23159872E-11 0.10181288E+05 0.49925659E+02 4

 AR 120186AR 1 G 0300.00 5000.00 1000.00 1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
 -0.07453750E+04 0.04366001E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366001E+02 4
 N2 Ranzi ON 2C 0H 0O OG 0300.00 5000.00 1000.00 1
 2.9266400E+00 1.4879770E-03 -5.6847603E-07 1.0097040E-10 -6.7533509E-15 2
 -922.76760E+00 5.9805290E+00 3.2986770E+00 1.4082399E-03 -3.9632218E-06 3
 5.6415148E-09 -2.4448540E-12 -1020.9000E00 3.9503720E+00 4
 HE Ranzi OHE 2C 0H 0O OG 0300.00 5000.00 1000.00 1
 3.1250000E+00 -1.4062505E-03 9.3750049E-07 -1.5625008E-10 0.0000000E+00 2
 -940.68700E+00 -2.4124130E+00 2.5000000E+00 0.0000000E+00 0.0000000E+00 3
 0.0000000E+00 0.0000000E+00 -745.37510E+00 0.9153489E+00 4
 B1O O 1 G 0300.00 5000.00 1000.00 1
 0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14 2
 0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04 3
 -0.01602843E-07 0.03890696E-11 0.02914764E+06 0.02963995E+02 4
 B2CO C 1O 1 G 0300.00 5000.00 1000.00 1
 0.03025078E+02 0.01442689E-01-0.05630828E-05 0.01018581E-08-0.06910952E-13 2
 -0.01426835E+06 0.06108218E+02 0.03262452E+02 0.01511941E-01-0.03881755E-04 3
 0.05581944E-07-0.02474951E-10-0.01431054E+06 0.04848897E+02 4
 B3C C 1 G 0300.00 5000.00 1000.00 1
 0.02602087E+02-0.01787081E-02 0.09087041E-06-0.01149933E-09 0.03310844E-14 2
 0.08542154E+06 0.04195177E+02 0.02498585E+02 0.08085777E-03-0.02697697E-05 3
 0.03040729E-08-0.01106652E-11 0.08545878E+06 0.04753459E+02 4
 B4CH C 1H 1 G 0300.00 5000.00 1000.00 1
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
 0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04 3
 0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331588E+02 4

B5CH2 CH2t C 1H 2 G 0300.00 5000.00 1000.00 1
 0.03636408E+02 0.01933057E-01-0.01687016E-05-0.01009899E-08 0.01808256E-12 2
 0.04534134E+06 0.02156561E+02 0.03762237E+02 0.01159819E-01 0.02489585E-05 3
 0.08800836E-08-0.07332435E-11 0.04536791E+06 0.01712578E+02 4
 B6CH2 CH2s C 1H 2 G 0300.00 5000.00 1000.00 1
 0.03552889E+02 0.02066788E-01-0.01914116E-05-0.01104673E-08 0.02021350E-12 2
 0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699089E-02 0.01025369E-04 3
 0.02492551E-07-0.01981266E-10 0.04989368E+06 0.05753207E+00 4
 H2 C 0H 2O 0 G 0300.00 5000.00 1000.00 1
 2.50170E+00 1.78083E-03 -7.80013E-07 1.48437E-10 -1.03401E-14 2
 -6.86891E+02 1.25553E+00 3.43853E+00 1.44314E-04 -1.08191E-07 3
 2.16839E-10 -5.54307E-14 -1.03749E+03 -3.92682E+00 4
 H2O C 0H 2O 1 G 0300.00 5000.00 1000.00 1
 2.68039E+00 3.09623E-03 -9.31393E-07 1.34865E-10 -7.70007E-15 2
 -2.99236E+04 6.77857E+00 3.97559E+00 -4.41834E-04 2.45596E-06 3
 -1.24431E-09 2.26702E-13 -3.02810E+04 7.71523E-02 4
 O2 C 0H 0O 2 G 0300.00 5000.00 1000.00 1
 3.19345E+00 1.56657E-03 -6.90657E-07 1.32082E-10 -9.23577E-15 2
 -1.05228E+03 5.96618E+00 3.08809E+00 1.60342E-03 -5.34550E-07 3
 2.80793E-11 2.98899E-15 -9.93828E+02 6.61069E+00 4
 H2O2 C 0H 2O 2 G 0300.00 5000.00 1000.00 1
 5.20269E+00 3.07820E-03 -8.47786E-07 1.14867E-10 -6.24436E-15 2
 -1.81737E+04 -2.81106E+00 2.79724E+00 9.30806E-03 -3.27081E-06 3
 -3.91853E-09 2.63341E-12 -1.75951E+04 9.47142E+00 4
 CH4 C 1H 4O 0 G 0300.00 5000.00 1000.00 1
 1.61991E+00 1.03080E-02 -3.71228E-06 6.14185E-10 -3.86748E-14 2
 -1.00748E+04 9.98982E+00 2.31954E+00 6.54738E-03 -7.48051E-07 3
 2.60912E-09 -1.95537E-12 -9.99764E+03 7.24965E+00 4
 HCHO MF-2011 C 1H 2O 1 G 0300.00 5000.00 1017.00 1
 2.9042036E+00 6.64407E-03 -2.45282E-06 4.12836E-10 -2.63040E-14 2
 -1.4432197E+04 7.5065143E+00 2.41049E+00 7.02041E-03 -4.22947E-06 3
 4.40116E-09 -2.12647E-12 -1.41114E+04 1.06246E+01 4
 CH3OH C 1H 4O 1 G 0300.00 5000.00 1000.00 1
 3.27626E+00 1.05432E-02 -3.54918E-06 5.58743E-10 -3.39236E-14 2
 -2.58917E+04 6.60656E+00 1.85957E+00 1.25312E-02 -4.47107E-06 3
 1.73293E-09 -8.71066E-13 -2.52879E+04 1.46835E+01 4
 CO2 C 1H 0O 2 G 0300.00 5000.00 1000.00 1
 2.73827E+00 6.09914E-03 -2.81755E-06 5.57282E-10 -3.99470E-14 2
 -4.82637E+04 8.67355E+00 2.67844E+00 6.31159E-03 1.20975E-06 3
 -7.46647E-09 3.79399E-12 -4.84134E+04 8.57691E+00 4
 CH3OOH C 1H 4O 2 G 0300.00 5000.00 1000.00 1
 6.37596E+00 1.07372E-02 -3.68666E-06 5.88827E-10 -3.61266E-14 2
 -1.84341E+04 -6.12840E+00 3.09218E+00 1.80223E-02 -7.11862E-06 3
 -1.47978E-09 1.45517E-12 -1.74300E+04 1.13028E+01 4
 C2H2 C 2H 2O 0 G 0300.00 5000.00 1000.00 1
 -0.11480273E+00 0.13168588E-01-0.61598394E-05 0.12302701E-08-0.88870914E-13 2
 0.27434125E+05 0.22531734E+02 0.23649659E+01 0.12770317E-01-0.10709240E-04 3
 0.34458529E-08 0.11729334E-12 0.26074828E+05 0.72850056E+01 4
 C2H4Z C 2H 4O 0 G 0300.00 5000.00 1000.00 1
 3.99720E-01 1.67299E-02 -6.80909E-06 1.22922E-09 -8.23928E-14 2
 5.63749E+03 1.97729E+01 1.31810E+00 1.44460E-02 -2.74335E-06 3
 -3.10835E-09 1.52772E-12 5.26817E+03 1.47233E+01 4

C2H6 C 2H 6O 0 G 0300.00 5000.00 1000.00 1
 3.94109E-01 2.11928E-02 -8.08560E-06 1.39339E-09 -9.03005E-14 2
 -1.10714E+04 1.96366E+01 9.75454E-01 1.88110E-02 -1.46453E-06 3
 -6.38247E-09 2.84067E-12 -1.13111E+04 1.65514E+01 4
 CH2COZ C 2H 2O 1 G 0300.00 5000.00 1000.00 1
 5.35267E+00 6.94209E-03 -2.50061E-06 4.13231E-10 -2.59692E-14 2
 -7.81007E+03 -3.80283E+00 2.99539E+00 1.23540E-02 -4.06499E-06 3
 -3.34608E-09 2.24152E-12 -7.15097E+03 8.53716E+00 4
 CH3CHO C 2H 4O 1 G 0300.00 5000.00 1000.00 1
 0.43235660E+01 0.13365114E-01-0.48470406E-05 0.80821411E-09-0.51297210E-13 2
 -0.22194609E+05 0.25847168E+01 0.27601621E+01 0.11889572E-01 0.67575984E-05 3
 -0.11965285E-07 0.41564356E-11-0.21409818E+05 0.12263453E+02 4
 C2H5OH C 2H 6O 1 G 0300.00 5000.00 1000.00 1
 5.62516E+00 1.59916E-02 -5.36799E-06 8.43422E-10 -5.11406E-14 2
 -3.10498E+04 -3.61961E+00 9.39858E-01 2.61811E-02 -9.25134E-06 3
 -3.45825E-09 2.62098E-12 -2.96238E+04 2.12634E+01 4
 C2H5OOH C 2H 6O 2 G 0300.00 5000.00 1000.00 1
 8.86549E+00 1.46991E-02 -4.66630E-06 7.03129E-10 -4.13262E-14 2
 -2.34663E+04 -1.74646E+01 2.03266E+00 3.20310E-02 -1.79773E-05 3
 2.38766E-09 1.07206E-12 -2.15063E+04 1.82187E+01 4
 CH3COOOH C 2H 4O 3 G 0300.00 5000.00 1000.00 1
 7.87651E+00 1.42400E-02 -4.81648E-06 7.62396E-10 -4.65514E-14 2
 -4.39851E+04 -9.71105E+00 2.19569E-01 3.53131E-02 -2.24276E-05 3
 3.22888E-09 1.67243E-12 -4.19548E+04 2.96617E+01 4

! DONNEES THERMODYNAMIQUES SUPPLEMENTAIRES !

! Ajout produits en C2+

C2H3CHO MF-BURCAT OC 3H 4O 1 G 0300.00 5000.00 1000.00 1
 8.20654919E+00 1.28492916E-02-4.64285331E-06 7.51738738E-10-4.51298116E-14 2
 -1.18838341E+04-1.49881933E+01 4.69868861E+00 4.99965957E-03 4.38587397E-05 3
 -6.12883900E-08 2.48508985E-11-1.00875286E+04 7.29812046E+00-8.18629119E+03 4
 CH2CHCO MF-BURCAT OC 3H 3O 1 G 0200.00 6000.00 1000.00 1
 7.69322269E+00 9.37928910E-03-3.31475709E-06 5.29225760E-10-3.14360567E-14 2
 8.15590313E+03-1.21011994E+01 3.13639619E+00 1.99890906E-02-7.99294937E-06 3
 -4.77227085E-09 3.89527783E-12 9.50725768E+03 1.18910245E+01 1.12526174E+04 4
 C3H2 OH 2C 3 O OG 0150.00 4000.00 1000.00 1
 7.67098100E+00 2.74874900E-03-4.37094300E-07-6.45559900E-11 1.66388700E-14 2
 6.25972200E+04-1.23689000E+01 3.16671400E+00 2.48257200E-02-4.59163700E-05 3
 4.26801900E-08-1.48215200E-11 6.35042100E+04 8.86944600E+00 4
 pC3H4 OC 3H 4 G 0300.00 5000.00 1000.00 1
 0.59767880E+01 0.11326920E-01-0.39663933E-05 0.64439298E-09-0.40119577E-13 2
 0.19653348E+05-0.83392105E+01 0.20619018E+01 0.20599686E-01-0.10556581E-04 3
 0.13453347E-08 0.47999533E-12 0.20849322E+05 0.12362522E+02 4
 aC3H4 OC 3H 4 G 0300.00 5000.00 1000.00 1
 0.61134343E+01 0.11383390E-01-0.40368400E-05 0.66247352E-09-0.41576704E-13 2
 0.20362814E+05-0.97686501E+01 0.11219990E+01 0.24131576E-01-0.14620023E-04 3
 0.33471641E-08 0.90883478E-13 0.21810221E+05 0.16326361E+02 4
 C3H6Y OC 3H 6 G 0300.00 5000.00 1000.00 1
 .50026493E+01 .17638993E-01 -.62266308E-05 .10151433E-08 -.63235977E-13 2
 -.27056152E+03 -.24723434E+01 .55598283E+00 .27091531E-01 -.10752104E-04 3
 -.97539210E-09 .14314721E-11 .11570190E+04 .21344173E+02 4

C3H8 OC 3H 8 G 0300.00 5000.00 1000.00 1
.54638848E+01 .22160569E-01 -.77296281E-05 .12495476E-08 -.77377605E-13 2
-.15629374E+05 -.62309151E+01 -.31831896E+00 .34746405E-01 -.12885018E-04 3
-.35057037E-08 .30165358E-11 -.13851594E+05 .24514595E+02 4
C4H2 OC 4H 2 G 0300.00 5000.00 1000.00 1
0.58399329E+01 0.11620689E-01-0.49604905E-05 0.92780533E-09-0.63876428E-13 2
0.54842219E+05-0.61394157E+01 0.41007705E+01 0.20304346E-01-0.14845920E-04 3
0.30114733E-08 0.76815767E-12 0.54847371E+05 0.12307835E+01 4
C4H4 OC 4H 4 G 0300.00 5000.00 1000.00 1
0.63549404E+01 0.15122039E-01-0.57226539E-05 0.98267505E-09-0.63638168E-13 2
0.33896547E+05-0.74671631E+01 0.15192467E+01 0.29964752E-01-0.19455949E-04 3
0.39837320E-08 0.64256348E-12 0.34997141E+05 0.16783657E+02 4
C4H6Z2 OC 4H 6 G 0300.00 5000.00 1000.00 1
.80518456E+01 .17540889E-01 -.61760657E-05 .10047656E-08 -.62479542E-13 2
.95697949E+04 -.18611710E+02 -.29224473E+00 .38725201E-01 -.16706719E-04 3
-.81080902E-08 .67421541E-11 .11749236E+05 .24444702E+02 4
cC4H6 OC 4H 6 G 0300.00 5000.00 1000.00 1
0.89762735E+01 0.17455665E-01-0.63610382E-05 0.10635568E-08-0.67594429E-13 2
0.24993229E+05-0.24260162E+02-0.23888779E+00 0.39345808E-01-0.22048607E-04 3
0.29083034E-08 0.10802864E-11 0.27801746E+05 0.24447674E+02 4
C4H6-12 OC 4H 6 G 0300.00 5000.00 1000.00 1
.88417616E+01 .15843917E-01 -.53288832E-05 .83887475E-09 -.50956042E-13 2
.15358018E+05 -.21569241E+02 .13161099E+01 .32781690E-01 -.17367984E-04 3
.31549054E-08 .24441525E-12 .17789736E+05 .18652039E+02 4
C4H6-1 OC 4H 6 G 0300.00 5000.00 1000.00 1
0.83276472E+01 0.16502315E-01-0.56312797E-05 0.89907620E-09-0.55341236E-13 2
0.16017064E+05-0.18720215E+02 0.14775175E+01 0.33041432E-01-0.18198547E-04 3
0.32913221E-08 0.41783853E-12 0.18094027E+05 0.17427605E+02 4
C4H6-2 OC 4H 6 G 0300.00 5000.00 1000.00 1
0.86370583E+01 0.15536721E-01-0.51298857E-05 0.80030371E-09-0.48487784E-13 2
0.13426500E+05-0.21647087E+02 0.19484946E+01 0.28219169E-01-0.11815486E-04 3
0.11804417E-08 0.25265242E-12 0.15847110E+05 0.15014225E+02 4
C4H8Y OC 4H 8 G 0300.00 5000.00 1000.00 1
0.93001947E+01 0.19871462E-01-0.65713975E-05 0.10258888E-08-0.62160394E-13 2
-0.46649707E+04-0.24260300E+02-0.25869742E+00 0.41475497E-01-0.21317686E-04 3
0.27918821E-08 0.85749311E-12-0.16180958E+04 0.26720718E+02 4
iC4H8 OC 4H 8 G 0300.00 5000.00 1000.00 1
0.10233544E+02 0.18412311E-01-0.59174949E-05 0.90512303E-09-0.54064721E-13 2
-0.69965908E+04-0.30797035E+02 0.87209290E+00 0.38349532E-01-0.18825667E-04 3
0.27373721E-08 0.43398726E-12-0.38566992E+04 0.19653683E+02 4
C4H7-2 OC 4H 7 G 0300.00 5000.00 1000.00 1
0.10921891E+02 0.13126064E-01-0.32941443E-05 0.41870504E-09-0.21872210E-13 2
0.22077002E+05-0.31360878E+02 0.19835423E+01 0.31981818E-01-0.18771878E-04 3
0.81298941E-08-0.21600354E-11 0.25246555E+05 0.17230307E+02 4
C4H7-1 OC 4H 7 G 0300.00 5000.00 1000.00 1
0.11142779E+02 0.13740587E-01-0.36293707E-05 0.48287518E-09-0.26251730E-13 2
0.19550055E+05-0.32037148E+02-0.12025269E+01 0.51008992E-01-0.50588929E-04 3
0.30729041E-07-0.82297173E-11 0.22993494E+05 0.31421394E+02 4
iC4H7 OC 4H 7 G 0300.00 5000.00 1000.00 1
0.11691871E+02 0.13670198E-01-0.36564963E-05 0.48932586E-09-0.26619352E-13 2
0.99949473E+04-0.37487293E+02 0.24674132E+00 0.40923573E-01-0.28221659E-04 3
0.11852519E-07-0.26292226E-11 0.13681498E+05 0.23464985E+02 4

C4H7Y MF-RODA C 4H 7O 0 G 0300.00 5000.00 1000.00 1
1.12103578e+01 1.60483196e-02-5.46502292e-06 8.45941053e-10-4.89772739e-14 2
1.09041937e+04-3.55593015e+01-3.50508352e-01 4.26511243e-02-2.90979373e-05 3
1.05403914e-08-1.60059854e-12 1.49933591e+04 2.67295696e+01 4
C4H7T OC 4H 7 G 0300.00 5000.00 1000.00 1
0.10011821E+02 0.14649572E-01-0.39018109E-05 0.51957955E-09-0.28117023E-13 2
0.23657344E+05-0.25818012E+02 0.46288908E+00 0.38231064E-01-0.26121455E-04 3
0.10982578E-07-0.22918540E-11 0.26659072E+05 0.24750271E+02 4
C4H10 OC 4H 10 G 0300.00 5000.00 1000.00 1
.77133317E+01 .27767614E-01 -.96156327E-05 .15456056E-08 -.95281279E-13 2
-.19425240E+05 -.16262451E+02 .59979584E-01 .44005580E-01 -.15532127E-04 3
-.52806315E-08 .40442116E-11 -.17040045E+05 .24565849E+02 4
C2H5CHO OC 3H 6O 1 G 0300.00 5000.00 1000.00 1
.70107722E+01 .18013448E-01 -.62295217E-05 .10005839E-08 -.61661722E-13 2
-.25691457E+05 -.95488281E+01 .28277023E+01 .25430365E-01 -.61913220E-05 3
-.50245177E-08 .26785609E-11 -.24271348E+05 .13234089E+02 4
CH3OCH3 OC 2H 6O 1 G 0300.00 5000.00 1000.00 1
.48582563E+01 .17240373E-01 -.59518788E-05 .95503494E-09 -.58825550E-13 2
-.24755031E+05 -.13852615E+01 .20368140E+01 .21299208E-01 -.51627690E-05 3
-.20305686E-08 .88250571E-12 -.23667908E+05 .14411049E+02 4
CH3OOCH3 OC 2H 6O 2 G 0300.00 5000.00 1000.00 1
.83690472E+01 .14833436E-01 -.46565133E-05 .69703088E-09 -.40832690E-13 2
-.18533230E+05 -.15578167E+02 .30638237E+01 .28614834E-01 -.24377980E-04 3
.19129631E-07 -.72663607E-11 -.16707926E+05 .12810528E+02 4
C3H7OH OC 3H 8O 1 G 0300.00 5000.00 1000.00 1
.71674681E+01 .22466624E-01 -.76292372E-05 .12097231E-08 -.73884075E-13 2
-.34686773E+05 -.95393562E+01 .12350693E+01 .34453284E-01 -.10589133E-04 3
-.54856804E-08 .35146994E-11 -.32804938E+05 .22268148E+02 4
C2H6CO OC 3H 6O 1 G 0300.00 5000.00 1000.00 1
.59975996E+01 .19679097E-01 -.70154574E-05 .11513579E-08 -.72035416E-13 2
-.29362656E+05 -.55254784E+01 .14577827E+01 .28063715E-01 -.90218518E-05 3
-.24536706E-08 .16730232E-11 -.27794104E+05 .19218454E+02 4
C3H8CO OC 4H 8O 1 G 0300.00 5000.00 1000.00 1
.87888947E+01 .24174010E-01 -.83446403E-05 .13376648E-08 -.82271822E-13 2
-.33018367E+05 -.17819489E+02 .27316518E+01 .35815358E-01 -.11085016E-04 3
-.44516226E-08 .28435873E-11 -.31006189E+05 .14949604E+02 4
iC4H3 C 4H 3O 0 G 0300.00 5000.00 1000.00 1
1.13140900E+01 5.01441400E-03-5.35044500E-07-2.82530900E-10 5.40327900E-14 2
5.18121100E+04-3.06243400E+01 6.54579900E+00 1.24247700E-02 5.60322600E-07 3
-5.63114100E-09 1.66521800E-12 5.35250300E+04-4.26408200E+00 4
nC4H3 C 4H 3O 0 G 0300.00 5000.00 1000.00 1
0.81544113E+01 0.84533300E-02-0.22554141E-05 0.30141167E-09-0.16387794E-13 2
0.62419848E+05-0.15504528E+02 0.13556120E+01 0.32820366E-01-0.35109366E-04 3
0.20636321E-07-0.50605436E-11 0.63911547E+05 0.18002588E+02 4
tC4H4 QB3-MF-11 OC 4H 4 G 0300.00 5000.00 1000.00 1
7.49703372E+00 1.34020744E-02-5.15621106E-06 9.12500005E-10-6.08955885E-14 2
3.63792351E+04-1.40628356E+01 1.02555769E+00 3.38766031E-02-3.08808670E-05 3
1.60366734E-08-3.49048890E-12 3.80855464E+04 1.88351771E+01 4
iC4H5 QB3-MF11 C 4H 5O 0 G 0300.00 5000.00 1000.00 1
8.22154969E+00 1.54731030E-02-5.94553320E-06 1.05135593E-09-7.01259575E-14 2
3.49969779E+04-1.75479573E+01-1.66166756E-01 4.18796377E-02-3.81388376E-05 3
1.87930486E-08-3.66766826E-12 3.71876785E+04 2.50572308E+01 4

nC4H5 C 4H 50 0 G 0300.00 5000.00 1000.00 1
0.87693729E+01 0.12676305E-01-0.35977159E-05 0.50347698E-09-0.28290782E-13 2
0.38532445E+05-0.19949425E+02-0.11109806E+01 0.46597324E-01-0.45865116E-04 3
0.23767367E-07-0.50623750E-11 0.40732270E+05 0.29018211E+02 4
C4H5-1s MF-Thergas C 4H 50 0 G 0300.00 5000.00 1000.00 1
0.97716198E+01 0.10864492E-01-0.28474749E-05 0.37631706E-09-0.20344954E-13 2
3.41090000E+04-0.24554909E+02 0.21635287E+01 0.31185936E-01-0.23202998E-04 3
0.97914157E-08-0.17814351E-11 3.63400000E+04 0.15158150E+02 4
C4H5-1p C 4H 50 0 G 0300.00 5000.00 1000.00 1
0.10232865E+02 0.10247763E-01-0.26092084E-05 0.33654396E-09-0.17835803E-13 2
0.39862383E+05-0.26845192E+02 0.56457460E+00 0.42366933E-01-0.46984671E-04 3
0.30757263E-07-0.85065835E-11 0.42355477E+05 0.21991501E+02 4
C4H5-2 MF-Thergas C 4H 50 0 G 0300.00 5000.00 1000.00 1
0.10349156E+02 0.96846446E-02-0.23720552E-05 0.29807440E-09-0.15556389E-13 2
3.28220000E+04-0.28037483E+02 0.11140869E+01 0.37001960E-01-0.39302799E-04 3
0.27354533E-07-0.82161031E-11 3.55850000E+04 0.19935490E+02 4
C6H2 C 6H 20 0 G 0300.00 5000.00 1000.00 1
2.09393E+01 -3.78743E-04 1.40024E-06 -3.82807E-10 3.20325E-14 2
5.47781E+04 -8.34171E+01 6.24203E+00 2.54433E-02 -9.25774E-06 3
-1.19041E-09 4.21126E-13 6.02411E+04 -2.21278E+00 4
IC6H4 C 6H 40 0 G 0300.00 5000.00 1000.00 1
2.09393E+01 -3.78743E-04 1.40024E-06 -3.82807E-10 3.20325E-14 2
5.47781E+04 -8.34171E+01 6.24203E+00 2.54433E-02 -9.25774E-06 3
-1.19041E-09 4.21126E-13 6.02411E+04 -2.21278E+00 4
IC6H6 C 6H 60 0 G 0300.00 5000.00 1000.00 1
1.30354E+01 1.84558E-02 -6.50404E-06 1.05888E-09 -6.58829E-14 2
3.66930E+04 -4.21936E+01 -1.37336E+00 5.44308E-02 -3.01877E-05 3
-1.98465E-09 5.08363E-12 4.07399E+04 3.29330E+01 4
IC6H8 MF-BURCAT C 6H 80 0 G 0200.00 6000.00 1000.00 1
0.13184588E+02 0.24023820E-01-0.86729021E-05 0.14049681E-08-0.84315805E-13 2
0.11858656E+05-0.45629943E+02 0.38587790E+01 0.15885821E-01 0.81120967E-04 3
-0.12184205E-06 0.50832636E-10 0.15950538E+05 0.10384627E+02 0.18307022E+05 4
!C6H4# C 6H 40 0 G 0300.00 5000.00 1000.00 1
!0.13753e+02 0.14800e-01 -0.59008e-05 0.10516e-08 -0.69939e-13 2
!0.37491e+05 -0.53710e+02 -0.29583e+01 0.61820e-01 -0.47172e-04 3
!0.10438e-07 0.14818e-11 0.41793e+05 0.31827e+02 4
C6H4# BENZYNE Burcat C 6H 40 0 G 0200.00 6000.00 1000.00 1
1.05707063E+01 1.56860613E-02-5.68267148E-06 9.22956737E-10-5.54966417E-14 2
5.04976657E+04-3.32563927E+01 7.21604591E-01 2.47976151E-02 3.16372209E-05 3
-6.53230986E-08 2.96082142E-11 5.39797980E+04 2.16733825E+01 5.54615216E+04 4
C6H6# C 6H 60 0 G 0300.00 5000.00 1000.00 1
0.87855539E+01 0.24007780E-01-0.89817968E-05 0.15290967E-08-0.98381555E-13 2
0.52728438E+04-0.27027435E+02-0.46098137E+01 0.58742289E-01-0.36557733E-04 3
0.59800462E-08 0.16549968E-11 0.90295186E+04 0.42635956E+02 4
C6H10# C 6H 100 0 G 0300.00 5000.00 1000.00 1
0.11050500E+02 0.32594997E-01-0.12011771E-04 0.20231115E-08-0.12917893E-12 2
-0.67873379E+04-0.38301155E+02-0.64386005E+01 0.77518739E-01-0.48530113E-04 3
0.97841397E-08 0.11553521E-11-0.17844912E+04 0.52936558E+02 4
C8H10# C 8H 100 0 G 0300.00 5000.00 1000.00 1
0.17088512E+02 0.28108800E-01-0.92846949E-05 0.14457705E-08-0.87311004E-13 2
-0.64339473E+04-0.68194397E+02-0.31023767E+01 0.72735257E-01-0.39950613E-04 3
0.66947181E-08 0.86978851E-12 0.16202747E+03 0.39996910E+02 4

C6H8# C 6H 80 0 G 0300.00 5000.00 1000.00 1
0.14348906E+02 0.22355305E-01-0.78442017E-05 0.12768860E-08-0.79641792E-13 2
0.65331211E+04-0.55479118E+02-0.19681283E+01 0.64869180E-01-0.42724627E-04 3
0.86322496E-08 0.12262384E-11 0.11120009E+05 0.29383038E+02 4
C2H4O#3 C 2H 40 1 G 0300.00 5000.00 1000.00 1
4.47758E+00 1.35869E-02 -5.00744E-06 8.41742E-10 -5.35809E-14 2
-8.75035E+03 -1.34619E+00 -9.24908E-01 2.64513E-02 -1.34725E-05 3
3.74058E-10 1.40310E-12 -7.13279E+03 2.71327E+01 4
R1H C 0H 10 0 G 0300.00 5000.00 1000.00 1
2.51382E+00 4.09189E-06 -2.41082E-09 5.71874E-13 -4.70917E-17 2
2.54654E+04 -5.34746E-01 2.51984E+00 -2.59920E-05 6.27898E-08 3
-6.29951E-11 2.23973E-14 2.54641E+04 -5.63259E-01 4
R2OH C 0H 10 1 G 0200.00 6000.00 1000.00 1
2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-15 2
3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-06 3
-3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01 4
R3OOH C 0H 10 2 G 0300.00 5000.00 1000.00 1
0.51959782E+01 0.81757625E-03-0.68517188E-07 0.35108038E-11-0.92723883E-16 2
-0.14855469E+02-0.34269409E+01 0.14628947E+01 0.13744416E-01-0.16368369E-04 3
0.90934318E-08-0.19818082E-11 0.81195471E+03 0.15048832E+02 4
R4CH3 C 1H 30 0 G 0300.00 5000.00 1000.00 1
1.02702E+00 9.49641E-03 -3.82860E-06 6.86498E-10 -4.57900E-14 2
1.67624E+04 1.53006E+01 2.94974E+00 5.11940E-03 -8.75334E-07 3
6.64224E-10 -5.42393E-13 1.61486E+04 5.05087E+00 4
R5CHO C 1H 10 1 G 0300.00 5000.00 1000.00 1
0.36094091E+01 0.28745262E-02-0.98788814E-06 0.15840323E-09-0.97735176E-14 2
0.32321035E+04 0.54304714E+01 0.35340273E+01 0.20234731E-02 0.51834081E-06 3
-0.37246076E-09-0.60802857E-13 0.33738574E+04 0.62388401E+01 4
R6CH2OH C 1H 30 1 G 0300.00 5000.00 1000.00 1
6.72615E+00 2.58400E-03 -3.43695E-07 2.58671E-11 -8.92075E-16 2
-5.93852E+03 -1.07401E+01 1.75181E+00 1.63562E-02 -2.19316E-05 3
2.01041E-08 -7.28744E-12 -4.21651E+03 1.57722E+01 4
R7CH3O C 1H 30 1 G 0300.00 5000.00 1000.00 1
6.45804E+00 3.22182E-03 -5.09801E-07 4.41966E-11 -1.69366E-15 2
-8.23233E+02 -1.22475E+01 2.40571E-01 1.87747E-02 -2.13180E-05 3
1.81151E-08 -6.61230E-12 1.35827E+03 2.11815E+01 4
R8CH3OO C 1H 30 2 G 0300.00 5000.00 1000.00 1
9.76413E+00 3.04276E-03 -4.67054E-07 3.87833E-11 -1.39425E-15 2
-1.91174E+03 -2.69241E+01 1.48937E+00 2.40776E-02 -2.38748E-05 3
1.51535E-08 -4.47557E-12 7.64340E+02 1.69852E+01 4
R9C2H C 2H 10 0 G 0300.00 5000.00 1000.00 1
0.40437493E+01 0.36123355E-02-0.95946029E-06 0.12793372E-09-0.69526612E-14 2
0.65947961E+05 0.19703522E+01 0.17718196E+01 0.17070146E-01-0.20073590E-04 3
0.88779526E-08-0.83304159E-12 0.65840078E+05 0.11053392E+02 4
R10C2H3V C 2H 30 0 G 0300.00 5000.00 1000.00 1
3.27253E+00 8.18550E-03 -2.26647E-06 3.09596E-10 -1.70006E-14 2
3.39897E+04 7.07663E+00 2.29441E+00 1.02693E-02 -3.45618E-06 3
3.18937E-10 6.99872E-14 3.43028E+04 1.23194E+01 4
R11C2H5 C 2H 50 0 G 0300.00 5000.00 1000.00 1
3.50261E+00 1.26143E-02 -3.65730E-06 5.16642E-10 -2.90469E-14 2
1.24032E+04 5.44236E+00 5.46580E-01 2.04368E-02 -1.16694E-05 3
4.82541E-09 -1.19281E-12 1.32743E+04 2.09001E+01 4

R12CHCOZ C 2H 10 1 G 0300.00 5000.00 1000.00 1
0.06758073E+02 0.02000400E-01-0.02027607E-05-0.01041132E-08 0.01965165E-12 2
0.01901513E+06-0.09071262E+02 0.05047965E+02 0.04453478E-01 0.02268283E-05 3
-0.01482095E-07 0.02250742E-11 0.01965892E+06 0.04818439E+01 4
R13CH2CHO MF-BURCAT C 2H 30 1 G 0200.00 6000.00 1000.00 1
6.53928338E+00 7.80238629E-03-2.76413612E-06 4.42098906E-10-2.62954290E-14 2
-1.18858659E+03-8.72091393E+00 2.79502600E+00 1.01099472E-02 1.61750645E-05 3
-3.10303145E-08 1.39436139E-11 1.62944975E+02 1.23646657E+01 1.53380440E+03 4
!coefficients de CHEMKIn a haute temperature et THERGAS a basse temperature!
R14CH3CO C 2H 30 1 G 0300.00 5000.00 1000.00 1
5.17844E+00 8.15192E-03 -2.10111E-06 2.71446E-10 -1.42897E-14 2
-5.94327E+03 -2.17361E-01 3.78076E+00 5.97858E-03 8.17510E-06 3
-8.25542E-09 1.81654E-12 -5.11877E+03 8.85731E+00 4
R15C2H5O C 2H 50 1 G 0300.00 5000.00 1000.00 1
8.79327E+00 8.37917E-03 -1.93446E-06 2.29371E-10 -1.13191E-14 2
-6.03107E+03 -2.23324E+01 -6.00093E-01 3.17670E-02 -2.42586E-05 3
1.08137E-08 -2.26856E-12 -3.08491E+03 2.73650E+01 4
R16C2H4OOH C 2H 50 2 G 0300.00 5000.00 1000.00 1
1.19639E+01 6.99398E-03 -1.39221E-06 1.46301E-10 -6.56315E-15 2
-1.64410E+02 -3.25611E+01 9.12805E-01 4.29306E-02 -5.09705E-05 3
3.45647E-08 -9.73011E-12 2.78459E+03 2.35878E+01 4
R17C2H5OO C 2H 50 2 G 0300.00 5000.00 1000.00 1
1.13253E+01 8.28625E-03 -1.86203E-06 2.18209E-10 -1.07868E-14 2
-6.98659E+03 -3.29488E+01 6.72056E-01 3.62757E-02 -3.00008E-05 3
1.38479E-08 -2.84583E-12 -3.78886E+03 2.28869E+01 4
R18CH3COOO C 2H 30 3 G 0300.00 5000.00 1000.00 1
1.10774E+01 6.59595E-03 -1.40685E-06 1.55610E-10 -7.22472E-15 2
-1.93998E+04 -2.93379E+01 -1.25738E+00 4.04124E-02 -3.66489E-05 3
1.70556E-08 -3.15366E-12 -1.58216E+04 3.48253E+01 4
R19C3H7 C 3H 70 0 G 0300.00 5000.00 1000.00 1
4.90850E+00 1.95492E-02 -6.09862E-06 9.08986E-10 -5.30994E-14 2
9.72711E+03 2.41566E-01 -9.97049E-01 4.22637E-02 -3.67683E-05 3
1.83985E-08 -3.66617E-12 1.08489E+04 2.87294E+01 4
R20C4H9 C 4H 90 0 G 0300.00 5000.00 1000.00 1
7.04485E+00 2.53221E-02 -8.04531E-06 1.21383E-09 -7.14512E-14 2
5.52642E+03 -9.13080E+00 -5.06119E-01 5.07221E-02 -3.74398E-05 3
1.45966E-08 -1.90079E-12 7.19571E+03 2.83231E+01 4
C3H3 C 3H 30 0 G 0300.00 5000.00 1000.00 1
0.78096647E+01 0.56143333E-02-0.12791088E-05 0.15269974E-09-0.77161059E-14 2
0.38026500E+05-0.16579403E+02 0.19126261E+01 0.23730382E-01-0.23743514E-04 3
0.13903455E-07-0.35110623E-11 0.39616629E+05 0.13564302E+02 4
sC3H5 H 5C 3 0 OG 0300.00 4000.00 1000.00 1
0.78482885E+01 0.95748352E-02-0.23817731E-05 0.30328015E-09-0.16003082E-13 2
0.28245344E+05-0.16577957E+02 0.37793621E+00 0.30234547E-01-0.27463551E-04 3
0.17104586E-07-0.49195583E-11 0.30526816E+05 0.22532042E+02 4
tC3H5 H 5C 3 0 OG 0300.00 4000.00 1000.00 1
.72541046E+01 .99584209E-02 -.24557530E-05 .30540118E-09 -.15559321E-13 2
.27536686E+05 -.12778450E+02 .12173898E+01 .24343655E-01 -.17027147E-04 3
.90219592E-08 -.24957287E-11 .29554811E+05 .19536684E+02 4
C3H5Y MF-RODA C 3H 50 0 G 0300.00 5000.00 1000.00 1
8.45883958e+00 1.12695483e-02-3.83792864e-06 5.94059119e-10-3.43918030e-14 2
1.63576092e+04-2.25809450e+01-5.29131958e-01 3.34559100e-02-2.53401027e-05 3

1.02865754e-08-1.73258340e-12 1.93834226e+04 2.53067131e+01 4
iC3H7 C 3H 70 0 G 0300.00 5000.00 1000.00 1
0.86707764E+01 0.13424351E-01-0.35232911E-05 0.46288709E-09-0.24745097E-13 2
0.71732666E+04-0.21719482E+02 0.43604645E+00 0.33385802E-01-0.21641390E-04 3
0.82326741E-08-0.13815982E-11 0.97955605E+04 0.22010902E+02 4
iC6H5 C 6H 50 0 G 0300.00 5000.00 1000.00 1
0.15886463E+02 0.10358742E-01-0.26210487E-05 0.33680408E-09-0.17818234E-13 2
0.64264773E+05-0.56288445E+02-0.65283889E+00 0.60272861E-01-0.56178018E-04 3
0.24491065E-07-0.39886753E-11 0.68454945E+05 0.27766666E+02 4
iC6H7 C 6H 70 0 G 0300.00 5000.00 1000.00 1
0.16082298E+02 0.14652845E-01-0.39246302E-05 0.52668248E-09-0.28757744E-13 2
0.42251578E+05-0.57395111E+02-0.18988532E+01 0.69014795E-01-0.62372797E-04 3
0.26989447E-07-0.44227855E-11 0.46797590E+05 0.33954002E+02 4
iC6H9 C 6H 90 0 G 0300.00 5000.00 1000.00 1
0.14508e+02 0.24775e-01 -0.80467e-05 0.12386e-08 -0.74237e-13 2
0.31903e+04 -0.48266e+02 -0.80809e+00 0.60717e-01 -0.34400e-04 3
0.59037e-08 0.96824e-12 0.79454e+04 0.32955e+02 4
C6H5# C 6H 50 0 G 0300.00 5000.00 1000.00 1
0.10562999E+02 0.17326031E-01-0.53726535E-05 0.80094376E-09-0.46991735E-13 2
0.35612875E+05-0.33390987E+02-0.35054851E+01 0.51216062E-01-0.28497903E-04 3
0.13292909E-08 0.27157382E-11 0.39760125E+05 0.40596451E+02 4
C6H7# C 6H 70 0 G 0300.00 5000.00 1000.00 1
0.16160069E+02 0.16076842E-01-0.46392893E-05 0.65612432E-09-0.37083770E-13 2
0.16631279E+05-0.63074673E+02-0.11001967E+01 0.60652319E-01-0.41787876E-04 3
0.99168647E-08 0.52658436E-12 0.21558750E+05 0.26926006E+02 4
C6H9Z# C 6H 90 0 G 0300.00 5000.00 1000.00 1
0.13230055E+02 0.25476102E-01-0.82115375E-05 0.12589454E-08-0.75337733E-13 2
0.31776328E+04-0.47774246E+02-0.56114020E+01 0.73584810E-01-0.48274313E-04 3
0.11749711E-07 0.21426784E-12 0.86383809E+04 0.50731293E+02 4
cC3H6 0C 3H 60 0G 0300.00 5000.00 1000.00 1
0.46943588E+01 0.19042941E-01-0.70509145E-05 0.11923079E-08-0.76385580E-13 2
0.36225312E+04-0.50023651E+01-0.31540399E+01 0.39798610E-01-0.23675864E-04 3
0.36800376E-08 0.11306161E-11 0.57714116E+04 0.35638264E+02 4
cC3H4 0C 3H 40 0G 0300.00 5000.00 1000.00 1
0.65029650E+01 0.11103593E-01-0.39504939E-05 0.64919903E-09-0.40751084E-13 2
0.30256143E+05-0.12088860E+02 0.13029232E+01 0.22985363E-01-0.11988642E-04 3
0.13175647E-08 0.63520624E-12 0.31892398E+05 0.15577282E+02 4
cC3H3 0C 3H 30 0G 0300.00 5000.00 1000.00 1
0.81922007E+01 0.54351720E-02-0.12350339E-05 0.14621292E-09-0.72950696E-14 2
0.49300547E+05-0.18844524E+02 0.18505306E+01 0.23016062E-01-0.21012138E-04 3
0.11653677E-07-0.29743033E-11 0.51160676E+05 0.14175776E+02 4
C5H9Y C 5H 90 0 G 0300.00 5000.00 1000.00 1
0.13169188E+02 0.19727064E-01-0.56167714E-05 0.78845036E-09-0.44429819E-13 2
0.70985156E+04-0.43151443E+02-0.78324392E-01 0.51707026E-01-0.33749246E-04 3
0.12455757E-07-0.23120414E-11 0.11270233E+05 0.27123213E+02 4
C5H8 C 5H 80 0 G 0300.00 5000.00 1000.00 1
0.11670992E+02 0.23878116E-01-0.88798688E-05 0.15070004E-08-0.96833511E-13 2
0.29606875E+04-0.38388065E+02 0.36735153E+01 0.31901374E-01-0.40754057E-05 3
-0.44839923E-08 0.10373115E-11 0.66159673E+04 0.81445122E+01 4
iC5H9 C 5H 90 0 G 0300.00 5000.00 1000.00 1
0.14801226E+02 0.19409005E-01-0.56848889E-05 0.81174234E-09-0.46132274E-13 2
0.14246453E+05-0.50913551E+02-0.52360737E+00 0.64075984E-01-0.58179972E-04 3

0.31737468E-07-0.78203676E-11 0.18559572E+05 0.28162197E+02 4
 iC5H8 C 5H 80 0 G 0300.00 5000.00 1000.00 1
 0.10759669E+02 0.22370014E-01-0.77185096E-05 0.12409445E-08-0.76699931E-13 2
 0.42152129E+04-0.31530663E+02-0.29550350E+00 0.53058356E-01-0.34172506E-04 3
 0.68792683E-08 0.10842018E-11 0.71024492E+04 0.25204750E+02 4
 C5H7Y C 5H 70 0 G 0300.00 5000.00 1000.00 1
 0.14042417E+02 0.17409818E-01-0.55104351E-05 0.83452856E-09-0.49549771E-13 2
 0.17833342E+05-0.50957664E+02 0.23821380E+01 0.38972169E-01-0.21452441E-04 3
 0.10172762E-07-0.33551931E-11 0.22353016E+05 0.13711008E+02 4
 iC5H7Y C 5H 70 0 G 0300.00 5000.00 1000.00 1
 0.12553609E+02 0.16907623E-01-0.49724572E-05 0.71237360E-09-0.40593282E-13 2
 0.19840184E+05-0.41390175E+02-0.93005651E+00 0.55704635E-01-0.43736953E-04 3
 0.16151073E-07-0.20300196E-11 0.23385055E+05 0.27688049E+02 4
 C5H10 C 5H 100 0 G 0300.00 5000.00 1000.00 1
 0.12413622E+02 0.24179598E-01-0.78829889E-05 0.12169197E-08-0.73090697E-13 2
 -0.86846465E+04-0.39354607E+02-0.37743804E+00 0.52917615E-01-0.27352471E-04 3
 0.35076957E-08 0.11387614E-11-0.45878291E+04 0.28933079E+02 4
 iC5H10 C 5H 100 0 G 0300.00 5000.00 1000.00 1
 0.12453186E+02 0.26599029E-01-0.93296321E-05 0.15186222E-08-0.94735763E-13 2
 -0.94587070E+04-0.41043900E+02 0.29573795E+00 0.55393700E-01-0.30924344E-04 3
 0.57856693E-08 0.57254977E-12-0.57005742E+04 0.23350286E+02 4
 C5H6# MF-Burcat C 5H 60 0 G 0300.00 5000.00 1000.00 1
 0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-13 2
 0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-04 3
 -0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02 0.16152485E+05 4
 iC5H9Y C 5H 90 0 G 0300.00 5000.00 1000.00 1
 0.12680129E+02 0.22156179E-01-0.68006971E-05 0.10050097E-08-0.58529800E-13 2
 0.53084492E+04-0.41084785E+02 0.25287175E+01 0.42894527E-01-0.17673357E-04 3
 -0.48191739E-09 0.17288109E-11 0.87291729E+04 0.13785473E+02 4
 C4H7V C 4H 70 0 G 0300.00 5000.00 1000.00 1
 0.10684196E+02 0.14119416E-01-0.37387376E-05 0.49625826E-09-0.26821481E-13 2
 0.24685330E+05-0.30063858E+02-0.39830261E+00 0.44143617E-01-0.36502337E-04 3
 0.18969859E-07-0.46769325E-11 0.27988551E+05 0.27853588E+02 4

!MECHANISM OF BENZENE

C4H4O MF-BURCAT C 4H 40 1 G 200.000 6000.00 1000.00 1
 9.74850463E+00 1.37125055E-02-5.05430099E-06 8.25446463E-10-4.97385204E-14 2
 -1.55172564E+03-2.40662801E+01 2.45069796E+00 2.60086795E-02 1.37550849E-06 3
 -2.17962924E-08 1.11438235E-11 8.71446510E+02 1.55762929E+01 2.73246650E+03 4
 iC5H6 OC 5H 6 G 0300.00 5000.00 1000.00 1
 0.11761186E+02 0.15722809E-01-0.52564237E-05 0.82627116E-09-0.50267011E-13 2
 0.25725818E+05-0.36669983E+02 0.60132211E+00 0.43948915E-01-0.28333196E-04 3
 0.64557306E-08 0.31841822E-12 0.28983785E+05 0.21763247E+02 4
 C5H4O# QB3-MF11 OC 5H 40 1 G 200.00 6000.00 1000.00 1
 1.05616223E+01 1.65688053E-02-6.50792182E-06 1.16944508E-09-7.89367301E-14 2
 2.66892704E+03-3.16898268E+01-3.39466227E+00 5.80284554E-02-5.15465249E-05 3
 2.11860929E-08-2.59810174E-12 6.39558887E+03 3.97191546E+01 4
 C5H5OH# MF-BURCAT OC 5H 60 1 G 0200.00 6000.00 1000.00 1
 1.16115218E+01 1.91901010E-02-6.83602335E-06 1.09795484E-09-6.55125692E-14 2
 -5.69452475E+03-3.68452441E+01 2.28105979E+00 1.72605889E-02 6.60492754E-05 3
 -1.06481809E-07 4.58889262E-11-1.99035320E+03 1.74654781E+01-1.48297975E+02 4
 C6H5OH# OC 6H 60 1G 0300.00 5000.00 1000.00 1

0.12198475E+02 0.22610646E-01-0.81984381E-05 0.13655722E-08-0.86539086E-13 2
-0.17240379E+05-0.40546387E+02-0.31016734E+01 0.64650230E-01-0.44300436E-04 3
0.92729806E-08 0.13425882E-11-0.13188701E+05 0.38161629E+02 4
OC6H4O QB3-MF11 OC 6H 4O 2G 0300.00 5000.00 1000.00 1
1.37660136E+01 1.95880964E-02-7.79038350E-06 1.41185019E-09-9.58706111E-14 2
-1.97017996E+04-4.68450500E+01-1.90967029E+00 6.27551691E-02-4.91753623E-05 3
1.54812327E-08-3.20924555E-13-1.53029253E+04 3.43114316E+01 4
C6H5CHO OC 7H 6O 1 G 0300.00 5000.00 1000.00 1
0.27822605E+02 0.62637692E-02-0.14661670E-05 0.18006827E-09-0.93566283E-14 2
-0.15845393E+05-0.12738686E+03-0.34431257E+01 0.66832952E-01-0.34990375E-04 3
0.32432945E-08 0.11444751E-11-0.46860913E+04 0.43472546E+02 4
toluene OC 7H 8O 0G 0300.00 5000.00 1000.00 1
0.11904304E+02 0.28934540E-01-0.10644716E-04 0.17906390E-08-0.11423150E-12 2
-0.34422266E+03-0.41137535E+02-0.48577561E+01 0.70124537E-01-0.43211745E-04 3
0.92291188E-08 0.55434552E-12 0.46851802E+04 0.47097549E+02 4
C6H5#C2H MF-BURCAT C 8H 6O 0 G 0200.00 6000.00 1000.00 1
1.63582907E+01 2.11974105E-02-7.65817215E-06 1.24134505E-09-7.45327960E-14 2
3.10375340E+04-6.22520227E+01-2.74707918E+00 7.78284438E-02-6.69709932E-05 3
2.37972496E-08-8.43279765E-13 3.61131008E+04 3.54221257E+01 3.82082350E+04 4
etC6H5 OC 8H 10O 0G 0300.00 5000.00 1000.00 1
0.15652943E+02 0.31103252E-01-0.10768533E-04 0.17365137E-08-0.10760791E-12 2
-0.42719316E+04-0.59025787E+02-0.44416370E+01 0.80284387E-01-0.48162310E-04 3
0.81840819E-08 0.17228618E-11 0.17186896E+04 0.46691605E+02 4
styrene OC 8H 8O 0G 0300.00 5000.00 1000.00 1
0.14527099E+02 0.28132908E-01-0.10051117E-04 0.16562113E-08-0.10413746E-12 2
0.10674016E+05-0.52857262E+02-0.36050019E+01 0.74985504E-01-0.48912687E-04 3
0.10911444E-07 0.75314467E-12 0.15848407E+05 0.41673645E+02 4
C6H5C3H3 OC 9H 8O 0G 0300.00 5000.00 1000.00 1
0.36883018E+02-0.39229947E-02 0.44785397E-05-0.11401402E-08 0.93646099E-13 2
0.19863391E+05-0.17474283E+03 0.64557141E+00 0.60461201E-01-0.21301958E-04 3
-0.50708819E-08 0.17910624E-11 0.33145441E+05 0.24968544E+02 4
C10H10# MF-BURCAT OC 10H 10O 0G 0200.00 6000.00 1000.00 1
1.96542923E+01 3.33886286E-02-1.20413130E-05 1.94963753E-09-1.16973259E-13 2
2.53473433E+04-8.08051980E+01 1.92659259E+00 2.78897531E-02 1.32941165E-04 3
-2.10257150E-07 9.03339117E-11 3.24585081E+04 2.27839249E+01 3.50742016E+04 4
biphenyl C 12H 10O 0 G 0300.00 5000.00 1000.00 1
0.19666628E+02 0.41563164E-01-0.15394864E-04 0.26053102E-08-0.16707561E-12 2
0.12096543E+05-0.81842010E+02-0.89908199E+01 0.11787912E+00-0.79417921E-04 3
0.16613194E-07 0.21431708E-11 0.19973012E+05 0.66565338E+02 4
!C5H5# OC 5H 5 G 0300.00 5000.00 1000.00 1
! 0.12041054E+02 0.12419174E-01-0.35119076E-05 0.49088300E-09-0.27598395E-13 2
! 0.25389121E+05-0.41311119E+02 0.11384680E+01 0.37457578E-01-0.21867269E-04 3
! 0.44332529E-08 0.24462607E-12 0.28850924E+05 0.16758369E+02 4
C5H5# T12/89C 5H 5 0 OG 300.00 2000.000 1000.00 1
0.74743938E+01 0.16012733E-01-0.64823148E-08-0.35819703E-08 0.92365071E-12 2
2.80860000E+04-0.16133000E+02 0.98349822E+00 0.33651476E-01-0.11054181E-06 3
-0.36743394E-07 0.23141184E-10 2.96260000E+04 0.16585519E+02 4
!C5H5# MF-BURCAT OC 5H 5 G 0300.00 5000.00 1000.00 1!H = 65.3 <Kern 1998>
! 1.02615305E+01 1.55578917E-02-5.54166182E-06 8.89865066E-10-5.30836089E-14 2
! 2.80714257E+04-2.92211926E+01 1.63934946E+00 1.69922044E-02 5.28961483E-05 3
! -9.02286424E-08 3.98154820E-11 3.13030941E+04 2.00912008E+01 3.17479394E+04 4
!C5H5 OC 5H 5 G 0300.00 5000.00 1000.00 1

0.13520258E+02 0.10585500E-01-0.27975798E-05 0.36991940E-09-0.19891141E-13 2
0.40809430E+05-0.46036358E+02-0.53843528E+00 0.49960259E-01-0.43163076E-04 3
0.18573136E-07-0.31771872E-11 0.44716559E+05 0.26607235E+02 4
C5H3O# QB3-MF-11 H 3C 5O 1 OG 300.00 5000.00 1000.00 1
1.06891340E+01 1.37493901E-02-5.44175193E-06 9.83039530E-10-6.66050286E-14 2
3.59108275E+04-3.06054496E+01-2.29545540E+00 5.35720933E-02-5.14929574E-05 3
2.42902334E-08-4.19455694E-12 3.93224094E+04 3.55416636E+01 4
C5H5O# MF-BURCAT OC 5H 5O 1 G 0200.00 6000.00 1000.00 1
1.20244667E+01 1.69698914E-02-6.12274609E-06 9.91737990E-10-5.95206422E-14 2
2.05122293E+04-3.95370458E+01 7.74871946E-01 2.53185105E-02 4.65761215E-05 3
-8.92691495E-08 4.04034749E-11 2.44938481E+04 2.34455624E+01 2.61043645E+04 4
C5H4OH# MF-BURCAT OC 5H 5O 1 G 0200.00 6000.00 1000.00 1
1.32735713E+01 1.53094185E-02-5.50115205E-06 8.88634759E-10-5.32324947E-14 2
2.27075873E+03-4.54766674E+01-1.74078500E+00 5.05423476E-02-1.59658908E-05 3
-2.73894335E-08 1.84710017E-11 6.52156699E+03 3.30332364E+01 8.06253742E+03 4
!C6H5O# C 6H 5O 1 G 0300.00 5000.00 1000.00 1
!0.13414198E+02 0.16568124E-01-0.49319242E-05 0.71277612E-09-0.40864390E-13 2
!-0.22550586E+03-0.46381676E+02-0.33557405E+01 0.61883949E-01-0.43446184E-04 3
!0.92753298E-08 0.13507817E-11 0.43056396E+04 0.40200157E+02 4
C6H5O# H 5C 6O 1 Og 300.00 5000.00 1000.00 1
1.23659442E+01 2.06807990E-02-8.15645830E-06 1.46982543E-09-9.94108782E-14 2
-5.19719088E+01-4.21156232E+01-4.15633912E+00 6.54916247E-02-4.80236259E-05 3
1.07615853E-08 2.14072559E-12 4.56697521E+03 4.34624876E+01 4
C6H4OH# OC 6H 5O 1 G 0300.00 5000.00 1000.00 1
0.13779563E+02 0.16367508E-01-0.48971697E-05 0.71227574E-09-0.41120438E-13 2
0.11955674E+05-0.47630394E+02-0.19387069E+01 0.56718133E-01-0.35267523E-04 3
0.36526806E-08 0.27459495E-11 0.16329568E+05 0.34105225E+02 4
C6H5O2 MF-BURCAT OC 6H 5O 2G 0200.00 6000.00 1000.00 1
1.53210095E+01 1.90635836E-02-6.90890063E-06 1.12266384E-09-6.75533163E-14 2
1.01192586E+04-5.54641890E+01 6.21315217E-01 3.87686270E-02 2.99476833E-05 3
-7.77124708E-08 3.69056482E-11 1.49950465E+04 2.49794441E+01 1.70318713E+04 4
OC6H4OH OC 6H 5O 2 G 0300.00 5000.00 1000.00 1
-0.28680062E+01 0.48046511E-01-0.20213529E-04 0.37413366E-08-0.25561183E-12 2
-0.14314042E+05 0.47972626E+02-0.32664216E+01 0.72835639E-01-0.57968322E-04 3
0.14403440E-07 0.23487022E-11-0.16911648E+05 0.40607937E+02 4
!MECHANISM OF TOLUENE
benzyl OC 7H 7O 0 G 0300.00 5000.00 1000.00 1
0.14451521E+02 0.22323409E-01-0.72202479E-05 0.11086372E-08-0.66355219E-13 2
0.17049973E+05-0.54730888E+02-0.47121730E+01 0.72093867E-01-0.52840940E-04 3
0.18332926E-07-0.22904658E-11 0.22674082E+05 0.45501709E+02 4
C6H4CH3 OC 7H 7O 0 G 0300.00 5000.00 1000.00 1
0.13686343E+02 0.22249535E-01-0.70373239E-05 0.10637213E-08-0.62992661E-13 2
0.28781602E+05-0.48606262E+02-0.35474486E+01 0.61160851E-01-0.31679134E-04 3
0.10949990E-08 0.28528477E-11 0.34182684E+05 0.43110756E+02 4
C6H4OHCO OC 7H 5O 2 G 0300.00 5000.00 1000.00 1
0.26250809E+02 0.89460416E-02-0.21397943E-05 0.26367367E-09-0.13549363E-13 2
-0.19938434E+05-0.11411957E+03-0.12110838E+01 0.61665673E-01-0.25545143E-04 3
-0.63137384E-08 0.47046152E-11-0.10333853E+05 0.35576443E+02 4
HOC6H4CH2OO OC 7H 7O 3 G 0300.00 5000.00 1000.00 1
0.11213660E+02 0.38049072E-01-0.14036586E-04 0.23677909E-08-0.15145173E-12 2
-0.12446613E+05-0.24645569E+02-0.41707492E+01 0.91290139E-01-0.70231959E-04 3
0.20282537E-07 0.22909756E-12-0.95057412E+04 0.50416073E+02 4

OC6H4CH3 OC 7H 70 1 G 0300.00 5000.00 1000.00 1
 0.73261833E+01 0.35739899E-01-0.13088922E-04 0.21956903E-08-0.13984673E-12 2
 -0.17064180E+04-0.10470680E+02-0.36008995E+01 0.72381422E-01-0.48228336E-04 3
 0.90683274E-08 0.23684448E-11 0.39322205E+03 0.43021164E+02 4
 HOC6H4CH2 OC 7H 70 1 G 0300.00 5000.00 1000.00 1
 0.82586975E+01 0.36033109E-01-0.13515761E-04 0.23064899E-08-0.14871879E-12 2
 -0.11910996E+04-0.16083267E+02-0.36051192E+01 0.79924382E-01-0.65464446E-04 3
 0.24912325E-07-0.28695943E-11 0.93602649E+03 0.41097092E+02 4
 C6H5CO OC 7H 50 1 G 0300.00 5000.00 1000.00 1
 0.26774740E+02 0.46817856E-02-0.78398284E-06 0.73234342E-10-0.30958701E-14 2
 0.56113867E+03-0.12106253E+03-0.22810972E+01 0.54210059E-01-0.15234797E-04 3
 -0.10887473E-07 0.49300798E-11 0.11423319E+05 0.39765499E+02 4
 C6H5CHOH OC 7H 70 1 G 0300.00 5000.00 1000.00 1
 1.02615305E+01 1.55578917E-02-5.54166182E-06 8.89865066E-10-5.30836089E-14 2
 2.69644257E+04-2.92211926E+01 1.63934946E+00 1.69922044E-02 5.28961483E-05 3
 -9.02286424E-08 3.98154820E-11 3.01960941E+04 2.00912008E+01 3.17479394E+04 4
 C6H5CH2O OC 7H 70 1 G 0300.00 5000.00 1000.00 1
 0.10762488E+02 0.30655593E-01-0.10738148E-04 0.17451247E-08-0.10868436E-12 2
 0.80504043E+04-0.30423080E+02-0.68475990E+01 0.81168644E-01-0.59274342E-04 3
 0.18262895E-07-0.10218114E-11 0.12635879E+05 0.59700500E+02 4
 HOC6H4CH2O OC 7H 70 2 G 0300.00 5000.00 1000.00 1
 0.86332483E+01 0.38273387E-01-0.14289769E-04 0.24314730E-08-0.15650075E-12 2
 -0.11905256E+05-0.14109512E+02-0.57563987E+01 0.88476494E-01-0.69227695E-04 3
 0.22478005E-07-0.11195157E-11-0.91235498E+04 0.56115089E+02 4
 C6H5CH2OO QB3-MF11 OC 7H 70 2 G 0300.00 5000.00 1000.00 1
 1.71115179E+01 2.68198282E-02-1.06205723E-05 1.91920856E-09-1.30061244E-13 2
 6.71623207E+03-6.12436900E+01-2.24622429E+00 7.26022303E-02-3.67327921E-05 3
 -8.74034681E-09 1.01564683E-11 1.24729027E+04 4.07042530E+01 4
 C8H9# OC 8H 90 0 G 0300.00 5000.00 1000.00 1
 0.16389204E+02 0.26334666E-01-0.81762873E-05 0.12212422E-08-0.71813351E-13 2
 0.12399031E+05-0.61402687E+02-0.31032555E+01 0.73243372E-01-0.44297161E-04 3
 0.92126609E-08 0.64196895E-12 0.18336816E+05 0.41555939E+02 4
 C8H9#-1 OC 8H 90 0 G 0300.00 5000.00 1000.00 1
 0.17974991E+02 0.23962518E-01-0.71549252E-05 0.10375772E-08-0.59694484E-13 2
 0.19424285E+05-0.69334557E+02-0.52652020E+01 0.88987760E-01-0.75449236E-04 3
 0.34149732E-07-0.66695443E-11 0.25960561E+05 0.50940002E+02 4
 C6H5C2H2 OC 8H 70 0 G 0300.00 5000.00 1000.00 1
 0.14594848E+02 0.23882853E-01-0.75691555E-05 0.11463872E-08-0.68014537E-13 2
 0.34474055E+05-0.52785233E+02-0.18172119E+01 0.60460128E-01-0.27423970E-04 3
 -0.40506389E-08 0.48146214E-11 0.39538484E+05 0.34447075E+02 4
 C14H13# OC 14H 130 OG 0300.00 5000.00 1000.00 1
 0.30027111E+02 0.38646519E-01-0.12025117E-04 0.17950720E-08-0.10530421E-12 2
 0.19811254E+05-0.13240137E+03-0.80962801E+01 0.13499202E+00-0.95191011E-04 3
 0.28873552E-07-0.22656774E-11 0.31146320E+05 0.67697067E+02 4
 !HOC6H4CH3 OC 7H 80 1 G 0300.00 5000.00 1000.00 1
 !0.51022620E+01 0.44136040E-01-0.18076045E-04 0.32825180E-08-0.22121157E-12 2
 !-0.18428398E+05 0.14670639E+01-0.34655142E+01 0.75982571E-01-0.51114544E-04 3
 !0.11117235E-07 0.16274848E-11-0.17099475E+05 0.42250137E+02 4
 HOC6H4CH3 BURCAT OC 7H 80 1 G 0300.00 5000.00 1000.00 1 !mf
 0.15932987E+02 0.27011160E-01-0.99448722E-05 0.16296689E-08-0.98513298E-13 2
 -0.23592065E+05-0.59732841E+02 0.42258267E+00 0.45551636E-01 0.32012513E-04 3
 -0.81121959E-07 0.37665658E-10-0.18202621E+05 0.26032903E+02-0.15911701E+05 4

C6H4OHCHO OC 7H 6O 2 G 0300.00 5000.00 1000.00 1
0.26727764E+02 0.11687560E-01-0.35472192E-05 0.52110433E-09-0.30284291E-13 2
-0.37618062E+05-0.11665517E+03-0.23217714E+01 0.73937416E-01-0.44468834E-04 3
0.69972113E-08 0.12057886E-11-0.27919160E+05 0.39755146E+02 4
C6H5CH2OH OC 7H 8O 1 G 0300.00 5000.00 1000.00 1
0.11269509E+02 0.37149373E-01-0.14254149E-04 0.24727249E-08-0.16134546E-12 2
-0.92585859E+04-0.28077469E+02-0.40976644E+01 0.81227809E-01-0.52230549E-04 3
0.90553014E-08 0.24712715E-11-0.54439961E+04 0.50132618E+02 4
C6H5CH2OOH OC 7H 8O 2 G 0300.00 5000.00 1000.00 1
0.11269509E+02 0.37149373E-01-0.14254149E-04 0.24727249E-08-0.16134546E-12 2
-0.92585859E+04-0.28077469E+02-0.40976644E+01 0.81227809E-01-0.52230549E-04 3
0.90553014E-08 0.24712715E-11-0.54439961E+04 0.50132618E+02 4
bibenzyl OC 14H 14O 0 G 0300.00 5000.00 1000.00 1
0.29121008E+02 0.43893188E-01-0.14857219E-04 0.23578921E-08-0.14450298E-12 2
0.31144297E+04-0.12893396E+03-0.83961201E+01 0.13422851E+00-0.81228864E-04 3
0.11706467E-07 0.40160093E-11 0.14418531E+05 0.68919365E+02 4
stilbene OC 14H 12O 0G 0300.00 5000.00 1000.00 1
0.27197937E+02 0.42290483E-01-0.14783480E-04 0.24010998E-08-0.14958465E-12 2
0.16200305E+05-0.11940059E+03-0.69465008E+01 0.12765117E+00-0.81015671E-04 3
0.14045111E-07 0.31788166E-11 0.26165121E+05 0.59502800E+02 4
!MECHANISM OF CYCLOPENTENE
C5H8# C 5H 8O 0 G 0300.00 5000.00 1000.00 1
4.03261E+00 3.27621E-02 -1.26209E-05 2.19041E-09 -1.42696E-13 2
8.71600E+02 1.97289E-01 -4.35697E+00 5.19141E-02 -2.18869E-05 3
-3.29975E-09 3.80784E-12 3.35629E+03 4.44739E+01 4
C5H8-12 C 5H 8O 0 G 0300.00 5000.00 1000.00 1
0.11842818E+02 0.20301070E-01-0.67252231E-05 0.10506498E-08-0.63661506E-13 2
0.11569117E+05-0.36193130E+02 0.63297063E+00 0.46450026E-01-0.26112299E-04 3
0.50091677E-08 0.41070825E-12 0.15082342E+05 0.23348232E+02 4
C5H7# C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.10825540E+02 0.18323712E-01-0.54506027E-05 0.78902423E-09-0.45379827E-13 2
0.19849064E+05-0.35182632E+02-0.43391600E+01 0.54159645E-01-0.35500372E-04 3
0.11872011E-07-0.17570134E-11 0.24683967E+05 0.45493938E+02 4
C5H7#Y C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.10627721E+02 0.18454375E-01-0.54704155E-05 0.78715573E-09-0.44934322E-13 2
0.13750512E+05-0.34146465E+02-0.38126223E+01 0.50147403E-01-0.27462424E-04 3
0.52330722E-08 0.23700302E-12 0.18507145E+05 0.43354416E+02 4
C5H7#V C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.10180723E+02 0.18947227E-01-0.56816752E-05 0.82814189E-09-0.47904324E-13 2
0.27145736E+05-0.31853241E+02-0.35276096E+01 0.46501085E-01-0.19530247E-04 3
-0.15096520E-08 0.22831049E-11 0.31811576E+05 0.42407509E+02 4
C5H7-1s C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.13535291E+02 0.14755227E-01-0.40365962E-05 0.55038296E-09-0.30397583E-13 2
0.36398219E+05-0.42910957E+02 0.10102913E+01 0.47329500E-01-0.37906382E-04 3
0.18942545E-07-0.46004975E-11 0.40241992E+05 0.22981096E+02 4
C5H7-2t C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.13085684E+02 0.14856261E-01-0.40114423E-05 0.53953303E-09-0.29395052E-13 2
0.35380070E+05-0.39796928E+02 0.75710320E+00 0.49347296E-01-0.45468300E-04 3
0.27554355E-07-0.77422417E-11 0.39070949E+05 0.24526548E+02 4
C5H7-4t C 5H 7O 0 G 0300.00 5000.00 1000.00 1
0.12619583E+02 0.14950674E-01-0.40118939E-05 0.53983290E-09-0.29568375E-13 2
0.32243912E+05-0.38948853E+02 0.75317645E+00 0.46317827E-01-0.34164801E-04 3

0.13351998E-07-0.21755779E-11 0.35703871E+05 0.22996468E+02 4
 C5H7-3t C 5H 7O 0 G 0300.00 5000.00 1000.00 1
 0.12345351E+02 0.18730117E-01-0.59229424E-05 0.89431101E-09-0.52875022E-13 2
 0.31284840E+05-0.42151211E+02 0.42308807E+01 0.24457168E-01 0.41350027E-05 3
 -0.84797280E-08 0.16412931E-11 0.35187812E+05 0.58466816E+01 4
 C5H7-5p C 5H 7O 0 G 0300.00 5000.00 1000.00 1
 0.11191008E+02 0.17708592E-01-0.51785605E-05 0.73931072E-09-0.42051235E-13 2
 0.37328652E+05-0.29865883E+02 0.64615750E+00 0.53074013E-01-0.52386011E-04 3
 0.31006643E-07-0.79222826E-11 0.39935824E+05 0.23094610E+02 4
 C5H7-12-5p C 5H 7O 0 G 0300.00 5000.00 1000.00 1
 0.13726429E+02 0.14088789E-01-0.37314239E-05 0.49567744E-09-0.26822135E-13 2
 0.35783562E+05-0.44248642E+02-0.24392813E+00 0.55519398E-01-0.54269291E-04 3
 0.31835043E-07-0.82835900E-11 0.39701082E+05 0.27711235E+02 4
 C5H9# C 5H 9O 0 G 0300.00 5000.00 1000.00 1
 9.04875E+00 2.67967E-02 -8.69665E-06 1.33362E-09 -7.94803E-14 2
 6.75857E+03 -2.50045E+01 -6.09849E+00 6.32478E-02 -3.48625E-05 3
 3.65881E-09 2.44852E-12 1.13153E+04 5.48538E+01 4
 C5H9 C 5H 9O 0 G 0300.00 5000.00 1000.00 1
 1.15745E+01 2.21084E-02 -6.56228E-06 9.42188E-10 -5.35366E-14 2
 1.66722E+04 -3.19960E+01 -8.85040E-01 5.90635E-02 -4.73812E-05 3
 2.08979E-08 -3.67432E-12 1.99957E+04 3.17793E+01 4
 MCP C 6H 10O 0 G 0300.00 5000.00 1000.00 1
 0.11536016E+02 0.32140490E-01-0.11846740E-04 0.19960575E-08-0.12750911E-12 2
 -0.53264746E+04-0.39499451E+02-0.40796714E+01 0.67783967E-01-0.37008485E-04 3
 0.59391412E-08 0.10267873E-11-0.36190686E+03 0.43704361E+02 4
 RMCP1 C 6H 9O 0 G 0300.00 5000.00 1000.00 1
 0.13873332E+02 0.24964714E-01-0.80716418E-05 0.12445720E-08-0.75006672E-13 2
 0.15452842E+05-0.50558205E+02-0.37768483E+01 0.67857273E-01-0.44802000E-04 3
 0.14575185E-07-0.19253230E-11 0.20937605E+05 0.42856590E+02 4
 RMCP2 C 6H 9O 0 G 0300.00 5000.00 1000.00 1
 0.14053507E+02 0.24486154E-01-0.78394123E-05 0.12010655E-08-0.72106268E-13 2
 0.18341211E+05-0.50915588E+02-0.49158297E+01 0.76581188E-01-0.64536289E-04 3
 0.32158336E-07-0.74590585E-11 0.23900064E+05 0.47900997E+02 4
 RMCPY1 C 6H 9O 0 G 0300.00 5000.00 1000.00 1
 0.13633660E+02 0.25172489E-01-0.81381741E-05 0.12538645E-08-0.75480082E-13 2
 0.93705625E+04-0.49290154E+02-0.32480927E+01 0.63820004E-01-0.36681195E-04 3
 0.78331199E-08 0.11149999E-12 0.14760687E+05 0.40709034E+02 4
 RMCPY2 C 6H 9O 0 G 0300.00 5000.00 1000.00 1
 0.13284031E+02 0.25177231E-01-0.80758009E-05 0.12374193E-08-0.74212514E-13 2
 0.95473730E+04-0.47591225E+02-0.35289767E+01 0.66731751E-01-0.46315534E-04 3
 0.18223426E-07-0.35650066E-11 0.14781354E+05 0.41324966E+02 4
 MCPD C 6H 8O 0 G 0300.00 5000.00 1000.00 1
 0.11055406E+02 0.26760619E-01-0.98032706E-05 0.16448022E-08-0.10477029E-12 2
 0.70527422E+04-0.35929955E+02-0.35884159E+01 0.65579586E-01-0.41417687E-04 3
 0.71932300E-08 0.17538306E-11 0.11066391E+05 0.39900093E+02 4
 RMCPD C 6H 7O 0 G 0300.00 5000.00 1000.00 1
 0.13601056E+02 0.19112684E-01-0.58309693E-05 0.85892521E-09-0.49962787E-13 2
 0.30698590E+05-0.47533340E+02-0.44133873E+01 0.74300565E-01-0.68765970E-04 3
 0.33237644E-07-0.66719573E-11 0.35327145E+05 0.44048241E+02 4
 RMCPDY C 6H 7O 0 G 0300.00 5000.00 1000.00 1
 0.12811765E+02 0.19838616E-01-0.60877323E-05 0.90033503E-09-0.52509432E-13 2
 0.19245729E+05-0.43404533E+02-0.31797397E+01 0.65515146E-01-0.53103620E-04 3

0.21857966E-07-0.36825083E-11 0.23557526E+05 0.38813900E+02 4
 anisole OC 7H 80 1 G 0300.00 5000.00 1000.00 1
 0.70653367E+01 0.40137362E-01-0.15948017E-04 0.28403546E-08-0.18907613E-12 2
 -0.13118277E+05-0.98643112E+01-0.58494267E+01 0.79079218E-01-0.52401600E-04 3
 0.12106050E-07 0.92676333E-12-0.10062839E+05 0.55265121E+02 4
 C6H5#OCH2 OC 7H 70 1 G 0300.00 5000.00 1000.00 1
 0.10423429E+02 0.30678995E-01-0.10676530E-04 0.17271368E-08-0.10722079E-12 2
 0.86203691E+04-0.25813568E+02-0.65495462E+01 0.86909175E-01-0.77541947E-04 3
 0.35875342E-07-0.66683451E-11 0.12541898E+05 0.58891670E+02 4
 bicycle H 5C 60 1 0g 300.00 5000.00 1000.00 1
 1.34330541E+01 1.95454051E-02-7.67763385E-06 1.37966440E-09-9.31263090E-14 2
 2.26264376E+04-4.62432675E+01-5.50271105E+00 7.95797700E-02-7.97489967E-05 3
 3.94054294E-08-7.19062542E-12 2.74673257E+04 4.96432974E+01 4
 (H)(CH3)C6H4O OC 7H 80 1 G 300.00 5000.00 1000.00 1
 1.41016511E+01 2.97645681E-02-1.16643059E-05 2.09193132E-09-1.40979030E-13 2
 -1.09963506E+04-4.94105742E+01-2.47699193E+00 7.00805378E-02-3.90178671E-05 3
 -4.89397681E-10 5.99177799E-12-6.06020347E+03 3.77733091E+01 4
 guaiacol OC 7H 80 2 G 200.000 6000.000 1000. 1
 1.74179969E+01 2.69660726E-02-9.77689109E-06 1.58515898E-09-9.51208998E-14 2
 -3.81712142E+04-6.51147424E+01 1.39819025E+00 4.75560316E-02 2.76747058E-05 3
 -7.56946077E-08 3.51628965E-11-3.26619145E+04 2.31758221E+01-3.00198087E+04 4
 HOC6H5#C2H5 H 10C 80 1 OG 300.00 5000.00 1000.00 1
 0.84541225E+01 0.46991013E-01-0.18390352E-04 0.32400207E-08-0.21400492E-12 2
 -0.22491801E+05-0.14385429E+02-0.34369209E+01 0.88062890E-01-0.60177921E-04 3
 0.14359378E-07 0.12226881E-11-0.20274684E+05 0.43511265E+02 4
 HOC6H5#C2H4 H 9C 80 1 OG 300.00 5000.00 1000.00 1
 0.98935471E+01 0.40589757E-01-0.14581622E-04 0.24135065E-08-0.15230632E-12 2
 -0.60218379E+04-0.21275200E+02-0.20276158E+01 0.80496632E-01-0.54944965E-04 3
 0.13905169E-07 0.70943858E-12-0.36449316E+04 0.37302074E+02 4
 HOstyrene H 8C 80 1 OG 300.00 5000.00 1000.00 1
 -0.96642151E+01 0.74756593E-01-0.34484267E-04 0.68241817E-08-0.48990927E-12 2
 -0.94589258E+03 0.85775330E+02-0.40545330E+01 0.89977846E-01-0.70576527E-04 3
 0.20145809E-07 0.12451855E-11-0.58128740E+04 0.44975578E+02 4
 !* MECHANISM OF INDANE (molecules)
 indane OC 9H 100 0 G 300.000 5000.000 1000.00 1
 1.49668322E+01 3.82114890E-02-1.50463379E-05 2.70759930E-09-1.82914939E-13 2
 -1.56895085E+03-5.96058726E+01-6.78373592E+00 8.53018482E-02-3.18013079E-05 3
 -2.19452546E-08 1.58027628E-11 5.15890865E+03 5.61157403E+01 4
 indene OC 9H 80 0 G 300.000 5000.000 1000.00 1
 1.53776039E+01 3.21363915E-02-1.26700376E-05 2.28233298E-09-1.54312315E-13 2
 1.08872191E+04-6.10238903E+01-7.49357917E+00 9.07281156E-02-5.76486055E-05 3
 4.69816415E-09 6.61632944E-12 1.74727480E+04 5.83347582E+01 4
 benzofuran OC 8H 60 1 G 200.000 6000.000 1000. 1 !Base Burcat!
 1.61267559E+01 2.42942790E-02-8.82919089E-06 1.43722155E-09-8.65592465E-14 2
 -5.74867958E+03-6.40564836E+01-7.85221476E-01 3.96432449E-02 5.69751746E-05 3
 -1.14831806E-07 5.19411145E-11 2.15748538E+02 3.02655928E+01 4
 ph#C3H5Z OC 9H 100 0 G 0300.00 5000.00 1000.00 1
 0.17334558E+02 0.32027453E-01-0.11025570E-04 0.17691381E-08-0.10916067E-12 2
 0.78309102E+04-0.65648361E+02-0.45074544E+01 0.84388874E-01-0.50438215E-04 3
 0.91186756E-08 0.14033403E-11 0.14489877E+05 0.49747856E+02 4
 ph#C3H5p OC 9H 100 0 G 0300.00 5000.00 1000.00 1
 0.18008806E+02 0.31342015E-01-0.10809463E-04 0.17442304E-08-0.10844952E-12 2

0.51716914E+04-0.70289879E+02-0.29644647E+01 0.82140356E-01-0.49615905E-04 3
 0.93745784E-08 0.12232701E-11 0.11507342E+05 0.40316849E+02 4
 ph#C3H7 OC 9H 120 0 G 0300.00 5000.00 1000.00 1
 0.19793148E+02 0.33311278E-01-0.11040036E-04 0.17237461E-08-0.10432178E-12 2
 -0.87604258E+04-0.79639320E+02-0.42074962E+01 0.89858957E-01-0.52841729E-04 3
 0.94316199E-08 0.14136324E-11-0.13302805E+04 0.47555656E+02 4
 ph#C4H9 OC 10H 140 0 G 0300.00 5000.00 1000.00 1
 0.22220839E+02 0.38906675E-01-0.12971250E-04 0.20348661E-08-0.12361402E-12 2
 -0.12587555E+05-0.90931335E+02-0.42641125E+01 0.10144480E+00-0.58435056E-04 3
 0.89912122E-08 0.22947432E-11-0.44398242E+04 0.49290642E+02 4
 cumene OC 9H 120 0 G 0300.00 5000.00 1000.00 1
 0.16221073E+02 0.39657544E-01-0.14122924E-04 0.23296629E-08-0.14701162E-12 2
 -0.77848418E+04-0.61098145E+02-0.52103133E+01 0.95287584E-01-0.59495935E-04 3
 0.11685747E-07 0.16412634E-11-0.17408159E+04 0.50435326E+02 4
 anisole OC 7H 80 1 G 0300.00 5000.00 1000.00 1
 0.70653367E+01 0.40137362E-01-0.15948017E-04 0.28403546E-08-0.18907613E-12 2
 -0.13118277E+05-0.98643112E+01-0.58494267E+01 0.79079218E-01-0.52401600E-04 3
 0.12106050E-07 0.92676333E-12-0.10062839E+05 0.55265121E+02 4
 C2H3C6H4CHO OC 9H 80 1 G 0300.00 5000.00 1000.00 1!thergas!
 0.25368549E+02 0.23065612E-01-0.80725604E-05 0.13141803E-08-0.82109361E-13 2
 -0.82031543E+04-0.10788841E+03-0.29223471E+01 0.85785232E-01-0.51136249E-04 3
 0.84651806E-08 0.13824329E-11 0.10018356E+04 0.43600605E+02 4
 CH3C6H4C3H7 OC 10H 140 0 G 0300.00 5000.00 1000.00 1!thergas!
 0.12677362E+02 0.54662075E-01-0.20537444E-04 0.35168519E-08-0.22773965E-12 2
 -0.95179766E+04-0.38002968E+02-0.44463081E+01 0.10469536E+00-0.66274552E-04 3
 0.14926529E-07 0.11421948E-11-0.52916499E+04 0.48972725E+02 4
 C9H8O# OC 9H 80 1 G 0300.00 5000.00 1000.00 1!Prof. Fournet
 1.68912777E+01 3.37594423E-02-1.33626483E-05 2.41352582E-09-1.63486545E-13 2
 -1.71100139E+04-6.66774238E+01-5.58628982E+00 8.74067911E-02-4.62813565E-05 3
 -6.27854330E-09 1.02002258E-11-1.04094257E+04 5.16787230E+01 4
 methylindane OC 10H 120 0 G 0300.00 5000.00 1000.00 1!Prof. Fournet
 1.67598011E+01 4.44775288E-02-1.74749149E-05 3.13956946E-09-2.11845862E-13 2
 -6.37162475E+03-6.79051820E+01-5.00066141E+00 8.57287318E-02-1.67723493E-05 3
 -3.94289200E-08 2.20695134E-11 6.82396380E+02 4.93884659E+01 4
 C2H3C6H4C2H5 OC 10H 120 0 G 0300.00 5000.00 1000.00 1!thergas!
 0.24699173E+02 0.30016012E-01-0.95521918E-05 0.14523023E-08-0.86466817E-13 2
 0.34377344E+03-0.10472086E+03-0.29563477E+01 0.97210743E-01-0.61970146E-04 3
 0.13299883E-07 0.92661436E-12 0.87100693E+04 0.41128498E+02 4
 C10H11 OC 10H 110 0 G 300.000 5000.000 1000.00 1!Cal
 1.76567421E+01 4.07422699E-02-1.60019384E-05 2.87442358E-09-1.93936508E-13 2
 1.15542700E+04-7.01419953E+01-5.49129163E+00 9.32521694E-02-4.13483528E-05 3
 -1.53461864E-08 1.39240207E-11 1.85979457E+04 5.24305846E+01 4
 C10H11-1 OC 10H 110 0 G 300.000 5000.000 1000.00 1!cal
 1.77163489E+01 4.07385733E-02-1.60139381E-05 2.87818716E-09-1.94265277E-13 2
 1.64174887E+04-7.07245973E+01-4.84443742E+00 9.04075314E-02-3.62051156E-05 3
 -1.95181541E-08 1.51977499E-11 2.33649486E+04 4.91279662E+01 4
 C10H11-2 OC 10H 110 0 G 300.000 5000.000 1000.00 1!Cal
 1.79682115E+01 4.03420610E-02-1.58175486E-05 2.83797111E-09-1.91319036E-13 2
 1.84380969E+04-7.24326681E+01-5.51415926E+00 9.55890834E-02-4.73499462E-05 3
 -9.78360661E-09 1.21124870E-11 2.54732733E+04 5.13932845E+01 4
 C10H11-3 OC 10H 110 0 G 300.000 5000.000 1000.00 1!Cal
 1.71601673E+01 4.13603158E-02-1.62826722E-05 2.92948852E-09-1.97871193E-13 2

1.03045132E+04-6.71864775E+01-5.31628896E+00 8.90340103E-02-3.10607127E-05 3
-2.47660001E-08 1.69889702E-11 1.73259090E+04 5.26889534E+01 4
C2H3C6H4CH2OH OC 9H 100 1 G 0300.00 5000.00 1000.00 1!thergas!
0.43951707E+01 0.57898611E-01-0.23767505E-04 0.43292485E-08-0.29271399E-12 2
-0.75151992E+04 0.10699394E+02-0.52335401E+01 0.96668668E-01-0.66096320E-04 3
0.15547579E-07 0.15935466E-11-0.63437466E+04 0.55395519E+02 4
C9H6O# OC 9H 60 1 G 0300.00 5000.00 1000.00 1!Prof. Fournet
1.70867721E+01 2.79042598E-02-1.10766291E-05 2.00494749E-09-1.36031879E-13 2
-1.20879155E+03-6.75684561E+01-6.07987619E+00 9.09556469E-02-6.85440546E-05 3
1.75776565E-08 1.80674746E-12 5.28359719E+03 5.24395569E+01 4
ph#C3H3 OC 9H 80 0 G 0300.00 5000.00 1000.00 1!thergas!
0.36992134E+02-0.41188644E-02 0.45946767E-05-0.11678456E-08 0.95939390E-13 2
0.19820523E+05-0.17534859E+03 0.32201937E+00 0.62704138E-01-0.26684971E-04 3
0.29608485E-09-0.10591397E-12 0.33180074E+05 0.26338909E+02 4
C8H8O# OC 8H 80 1 G 0300.00 5000.00 1000.00 1!Prof. Fournet
1.50839842E+01 3.25092066E-02-1.28403261E-05 2.31578474E-09-1.56702946E-13 2
-1.33912799E+04-5.85151857E+01-5.96220908E+00 8.15010579E-02-3.93920844E-05 3
-1.07682941E-08 1.14611472E-11-7.06811930E+03 5.25774976E+01 4
ph#C4H5 OC 10H 100 0 G 0300.00 5000.00 1000.00 1!thergas!
0.43195259E+02-0.50415727E-02 0.56516437E-05-0.14374750E-08 0.11810283E-12 2
0.14121508E+05-0.20917856E+03 0.60781814E-01 0.72740965E-01-0.29047997E-04 3
-0.17011532E-08 0.59878995E-12 0.29901045E+05 0.28318855E+02 4
ph#C3H4OH-1 OC 9H 100 1 G 0300.00 5000.00 1000.00 1!thergas!
0.42698853E+02-0.51612635E-02 0.56768863E-05-0.14359754E-08 0.11773621E-12 2
-0.22525232E+05-0.20329214E+03-0.49856192E+00 0.72838694E-01-0.29239585E-04 3
-0.16092433E-08 0.56729925E-12-0.67355664E+04 0.34508671E+02 4
ph#C3H4OH-2 OC 9H 100 1 G 0300.00 5000.00 1000.00 1!thergas!
-0.66692920E+01 0.77372409E-01-0.34142504E-04 0.65458803E-08-0.45919301E-12 2
-0.24562461E+04 0.71619812E+02-0.55595193E+01 0.10143711E+00-0.74890726E-04 3
0.19966048E-07 0.15351409E-11-0.57695332E+04 0.55291218E+02 4
C6H4C3H4 OC 9H 80 0 G 0300.00 5000.00 1000.00 1!thergas!
0.16345461E+02 0.30081328E-01-0.11020207E-04 0.18535914E-08-0.11852116E-12 2
0.28237611E+05-0.62544449E+02-0.24291337E+01 0.79446889E-01-0.52616906E-04 3
0.11910263E-07 0.80573108E-12 0.33495973E+05 0.34995358E+02 4
C3H5C6H4CH3 OC 10H 120 0 G 0300.00 5000.00 1000.00 1!thergas!
-0.39402735E+01 0.78336917E-01-0.33676853E-04 0.63375358E-08-0.43861610E-12 2
0.10209666E+05 0.54373463E+02-0.43788743E+01 0.10349764E+00-0.72757903E-04 3
0.18460829E-07 0.16557064E-11 0.76452373E+04 0.47218334E+02 4
methylindene-2 H 10C 10 0 0g 300.00 5000.00 1000.00 1!Prof.Fournet
1.68381088E+01 3.87904850E-02-1.52694162E-05 2.74719664E-09-1.85566081E-13 2
5.09511954E+03-6.72533365E+01-6.03745507E+00 9.13652746E-02-4.26934230E-05 3
-1.24523994E-08 1.26537842E-11 1.20277308E+04 5.37246453E+01 4

!* MECHANISM OF INDANE (free radicals)

indanyl-Y OC 9H 90 0 G 0300.00 5000.00 1000.00 1
1.58195435E+01 3.45357901E-02-1.36013494E-05 2.44804520E-09-1.65409696E-13 2
1.62783704E+04-6.19015515E+01-7.07869380E+00 9.13681374E-02-5.31256325E-05 3
-8.66380926E-10 8.66347995E-12 2.29720325E+04 5.80700378E+01 4
indanyl-1 OC 9H 90 0 G 0300.00 5000.00 1000.00 1
1.59473355E+01 3.45022437E-02-1.36104873E-05 2.45235218E-09-1.65824276E-13 2
2.10368722E+04-6.27284641E+01-6.39255004E+00 8.90927473E-02-4.99147282E-05 3

-2.81253096E-09 9.07608752E-12 2.76245796E+04 5.45646593E+01 4
C2H3C6H4CH2 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1
1.70648122E+01 3.28892095E-02-1.28323249E-05 2.29479720E-09-1.54348164E-13 2
2.48599234E+04-6.61223497E+01-5.67362805E+00 9.67482623E-02-7.49811328E-05 3
2.31114824E-08-1.30018265E-14 3.11297550E+04 5.11628285E+01 4
C3H5C6H4 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1
1.62351320E+01 3.39370160E-02-1.33112454E-05 2.38904749E-09-1.61096310E-13 2
3.90232459E+04-5.97461068E+01-4.32960560E+00 8.32985856E-02-4.38178187E-05 3
-5.70629532E-09 9.57164305E-12 4.51286697E+04 4.84374340E+01 4
C6H4C2H3 OC 8H 7O 0 G 0300.00 5000.00 1000.00 1 !thergas!
0.16176041E+02 0.21759402E-01-0.66688217E-05 0.98414743E-09-0.57243313E-13 2
0.41049367E+05-0.59604996E+02-0.23101082E+01 0.66132776E-01-0.37655747E-04 3
0.30604628E-08 0.29490531E-11 0.46557465E+05 0.37769215E+02 4
CH3C6H4C3H6 OC 10H 13O 0 G 0300.00 5000.00 1000.00 1 !thergas!
0.15751234E+02 0.45884017E-01-0.15792721E-04 0.25429037E-08-0.15777966E-12 2
0.14303363E+05-0.52437325E+02-0.52154360E+01 0.11301257E+00-0.92615024E-04 3
0.39931479E-07-0.69055352E-11 0.19315596E+05 0.52901985E+02 4
C9H9O# OC 9H 9O 1 G 0300.00 5000.00 1000.00 1!Prof. Fournet
1.77394753E+01 3.57991458E-02-1.41613150E-05 2.55662502E-09-1.73121736E-13 2
4.80796438E+03-7.18678743E+01-6.97808501E+00 9.68902592E-02-5.62370334E-05 3
-1.40681844E-09 9.41150780E-12 1.20512280E+04 5.77131836E+01 4
C2H3C6H4CH2O OC 9H 9O 1 G 0300.00 5000.00 1000.00 1 !thergas!
0.67678118E+01 0.50415479E-01-0.19377434E-04 0.33717502E-08-0.22081268E-12 2
0.17591494E+05-0.30051651E+01-0.65153575E+01 0.10028169E+00-0.75823082E-04 3
0.23908285E-07-0.94255094E-12 0.19766990E+05 0.60443253E+02 4
C3H5C6H4O OC 9H 9O 1 G 0300.00 5000.00 1000.00 1 !thergas!
0.88563671E+01 0.45847762E-01-0.16957136E-04 0.28722236E-08-0.18459954E-12 2
0.85710645E+04-0.12922363E+02-0.42699232E+01 0.92072673E-01-0.64674867E-04 3
0.15971544E-07 0.12960735E-11 0.10919846E+05 0.50648186E+02 4
C9H7O# OC 9H 7O 1 G 0300.00 5000.00 1000.00 1Prof. Fournet
1.78410949E+01 2.99865857E-02-1.18797738E-05 2.14734438E-09-1.45548004E-13 2
1.97341642E+04-7.10881494E+01-6.81388737E+00 9.65745085E-02-7.07151877E-05 3
1.55337451E-08 3.30073948E-12 2.66471435E+04 5.66996625E+01 4
ph#C3H2 OC 9H 7O 0 G 0300.00 5000.00 1383.00 1
0.13230577E+02 0.33664186E-01-0.12504979E-04 0.21206936E-08-0.13620751E-12 2
0.30061271E+05-0.42513824E+02-0.32099228E+01 0.78699686E-01-0.51982599E-04 3
0.12151481E-07 0.68123437E-12 0.34472039E+05 0.42208481E+02 4
ph#C3H6-1 OC 9H 11O 0 G 0300.00 5000.00 1000.00 1
0.21838772E+02 0.26736012E-01-0.77973918E-05 0.11125123E-08-0.63333521E-13 2
0.15403531E+05-0.88539001E+02-0.49415665E+01 0.97933039E-01-0.78598059E-04 3
0.33853315E-07-0.64276492E-11 0.23273246E+05 0.51333801E+02 4
ph#C3H4Y OC 9H 9O 0 G 0300.00 5000.00 1000.00 1
0.18109861E+02 0.27004687E-01-0.83208515E-05 0.12363505E-08-0.72453172E-13 2
0.20150484E+05-0.68283104E+02-0.40561695E+01 0.83991505E-01-0.61489729E-04 3
0.23307877E-07-0.38069652E-11 0.26775083E+05 0.48008499E+02 4
ph#C3H4-1 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1 !thergas!
0.18975496E+02 0.25666995E-01-0.77599279E-05 0.11396812E-08-0.66376090E-13 2
0.37120199E+05-0.72848488E+02-0.46363945E+01 0.86889327E-01-0.65126973E-04 3
0.24760910E-07-0.39351005E-11 0.44111707E+05 0.50811314E+02 4
ph#C3H4-2 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1 !thergas!
0.18543642E+02 0.25734363E-01-0.77141658E-05 0.11244412E-08-0.65064145E-13 2
0.36096484E+05-0.69826035E+02-0.48555102E+01 0.88737167E-01-0.72353097E-04 3

0.33076102E-07-0.69800550E-11 0.42935629E+05 0.52204437E+02 4
ph#C3H4-3 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1!thergas!
0.18248596E+02 0.26675191E-01-0.81630187E-05 0.12065303E-08-0.70427537E-13 2
0.28671299E+05-0.70557983E+02-0.21714995E+01 0.74953400E-01-0.44746736E-04 3
0.93193604E-08 0.52616228E-12 0.34999336E+05 0.37659279E+02 4
ph#C3H4-4 OC 9H 9O 0 G 0300.00 5000.00 1000.00 1!thergas!
0.19464947E+02 0.24629079E-01-0.72619359E-05 0.10433868E-08-0.59635206E-13 2
0.33433941E+05-0.75880455E+02-0.32146115E+01 0.85730106E-01-0.69593072E-04 3
0.31319615E-07-0.64286671E-11 0.40044785E+05 0.42349106E+02 4
indenyl OC 9H 7O 0 G 300.000 5000.000 1000. 1
1.59706473E+01 2.86651352E-02-1.12949950E-05 2.03414690E-09-1.37519923E-13 2
2.48192174E+04-6.29027317E+01-8.19315997E+00 9.69513671E-02-7.78644905E-05 3
2.41142048E-08 1.64713468E-13 3.14272288E+04 6.15513565E+01 4
naphthyl OC 10H 7O 0 G 200.000 6000.000 1000. 1!Base burcat!
1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14 2
3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
-9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4
C8H7O# OC 8H 7O 1 G 0300.00 5000.00 1000.00 1!thergas!
0.39498155E+01 0.47736809E-01-0.19333373E-04 0.34884815E-08-0.23430105E-12 2
0.10867305E+05-0.46506844E+01-0.64320035E+01 0.91989711E-01-0.72167728E-04 3
0.22816783E-07-0.66101562E-12 0.11987392E+05 0.42892570E+02 4
C8H7O#-1 OC 8H 7O 1 G 0300.00 5000.00 1000.00 1!thergas!
0.36577377E+01 0.48040181E-01-0.19457286E-04 0.35114045E-08-0.23589068E-12 2
0.52084609E+04-0.30909843E+01-0.60815744E+01 0.89198485E-01-0.67060450E-04 3
0.19099829E-07 0.30027036E-12 0.62320034E+04 0.41498894E+02 4
ph#C3H6-Y OC 9H 11O 0 G 0300.00 5000.00 1000.00 1!thergas
0.20312992E+02 0.28807884E-01-0.86748423E-05 0.12716173E-08-0.74028674E-13 2
0.80781914E+04-0.80869186E+02-0.38688006E+01 0.90247162E-01-0.65779976E-04 3
0.25497407E-07-0.44571040E-11 0.15395556E+05 0.46306519E+02 4
ph#C3H6-2 OC 9H 11O 0 G 0300.00 5000.00 1000.00 1!thergas
0.21145403E+02 0.27397629E-01-0.80628479E-05 0.11625580E-08-0.66916192E-13 2
0.14561053E+05-0.84495888E+02-0.43664527E+01 0.94754837E-01-0.74765012E-04 3
0.32140218E-07-0.61739290E-11 0.22105348E+05 0.48928509E+02 4
C3H5C6H4CH2 OC 10H 11O 0 G 0300.00 5000.00 1000.00 1!thergas!
-0.85401887E+00 0.69693714E-01-0.28514492E-04 0.51829545E-08-0.34997192E-12 2
0.28195023E+05 0.38386494E+02-0.47099199E+01 0.10417885E+00-0.77969838E-04 3
0.23642379E-07-0.71247587E-13 0.26622865E+05 0.49041828E+02 4
indenyl-2 H 7C 9 0 Og 300.00 5000.00 1000.00 1!Prof.Fournet
1.54934859E+01 2.92933033E-02-1.15860097E-05 2.09172056E-09-1.41651188E-13 2
4.39737207E+04-5.99761383E+01-6.58113902E+00 8.66716791E-02-5.76018051E-05 3
7.25729584E-09 5.33782120E-12 5.02874581E+04 5.50201049E+01 4
indenyl-3 H 7C 9 0 Og 300.00 5000.00 1000.00 1!Prof.Fournet
1.55336759E+01 2.92535025E-02-1.15699429E-05 2.08877913E-09-1.41450021E-13 2
4.37936144E+04-6.02768350E+01-6.79842164E+00 8.82352398E-02-6.11040498E-05 3
1.05524282E-08 4.21204227E-12 5.01366533E+04 5.58359657E+01 4
naphtol HR 6/99 BLYP C 10H 8O 1 OG 300.000 5000.000 1395.000 01!NOUVEAU
2.61461217E+01 2.46035266E-02-8.61118350E-06 1.35779500E-09-7.96351828E-14 2
-1.62253653E+04-1.17940723E+02-7.42523947E+00 1.15882243E-01-1.06394867E-04 3
4.96248553E-08-9.19061783E-12-5.79458155E+03 5.78975921E+01 4
naphtol-2 HR 6/99 BLYP C 10H 8O 1 OG 300.000 5000.000 1394.000 01!NOUVEAU
2.60758935E+01 2.46910885E-02-8.64754101E-06 1.36410864E-09-8.00285533E-14 2
-1.61139144E+04-1.18755598E+02-8.31179579E+00 1.19635782E-01-1.12084722E-04 3

5.32313499E-08-1.00013101E-11-5.54787579E+03 6.08896927E+01 4
A2O HR 6/99 BLYP C 10H 7O 1 OG 300.000 5000.000 1401.000 01!NOUVEAU
2.55199785E+01 2.25375617E-02-7.79622686E-06 1.22014387E-09-7.12043903E-14 2
-9.13287721E+02-1.15169184E+02-7.45889821E+00 1.10408595E-01-9.86444941E-05 3
4.41246608E-08-7.80459565E-12 9.35231821E+03 5.79329757E+01 4
C5H4CCH2 cbd-qb3 pag C 7H 6 O OG 300.000 5000.000 1396.000 1!by Dr. Glaude
1.68121948E+01 1.68679712E-02-5.85620989E-06 9.18454953E-10-5.36680000E-14 2
3.60029314E+04-6.67439600E+01-3.88857913E+00 7.16285896E-02-6.27290636E-05 3
2.81593703E-08-5.06188863E-12 4.25632251E+04 4.21812285E+01 4
C5H5CCH cbd-qb3 pag C 7H 6 O OG 300.000 5000.000 1397.000 1!by Dr. Glaude
1.68972508E+01 1.67331982E-02-5.79543147E-06 9.07443659E-10-5.29640367E-14 2
4.09232497E+04-6.70082451E+01-3.90528821E+00 7.27894554E-02-6.51288475E-05 3
2.98127578E-08-5.44054969E-12 4.74164546E+04 4.20935797E+01 4
chrysene OC 18H 12O 0 G 0300.00 5000.00 1673.00 1!Slavinskaya09,Richter2000
3.31662137E+01 5.08795514E-02-1.87182202E-05 3.06104765E-09-1.84366391E-13 2
1.57642287E+04-1.59238481E+02 3.12629742E+00 1.06385095E-01-4.82700462E-05 3
5.22816930E-09 1.05961625E-12 2.69644034E+04 6.40602579E+00 4
antra C 14H 10O 0 G 0300.00 5000.00 1000.00 1!DHf=55kcal au lie de 52kcal
0.65277452E+01 0.72339669E-01-0.30853811E-04 0.57675882E-08-0.39692292E-12 2
0.22804185E+05-0.10611534E+02-0.85285759E+01 0.12767017E+00-0.88071676E-04 3
0.19813367E-07 0.25009834E-11 0.25325042E+05 0.62289558E+02 4
ph#C4H7-3 OC 10H 12O 0 G 0300.00 5000.00 1000.00 1!trans
0.21045616E+02 0.35668906E-01-0.12075875E-04 0.19165953E-08-0.11745399E-12 2
0.12067930E+04-0.85048279E+02-0.41100893E+01 0.96507579E-01-0.56764144E-04 3
0.78674329E-08 0.29018394E-11 0.87476797E+04 0.47488205E+02 4
ph#C4H8X OC 10H 13O OG 0300.00 5000.00 1000.00 1
0.22983511E+02 0.33949055E-01-0.10327632E-04 0.15168742E-08-0.87988143E-13 2
0.41329570E+04-0.93396637E+02-0.38836262E+01 0.10158699E+00-0.70856317E-04 3
0.24595296E-07-0.34271785E-11 0.12255588E+05 0.47963360E+02 4
CH3phenanth OC 15H 12O 0 G 300.00 5000.00 2025.00 1!Slavinskaya09,Richter2000
2.86721901E+01 4.57935671E-02-1.67466881E-05 2.72794395E-09-1.63863026E-13 2
6.77859249E+03-1.31269124E+02 2.45407326E-01 1.03437006E-01-5.52427842E-05 3
1.17708807E-08-4.92994185E-13 1.69368456E+04 2.37077261E+01 4
CH2phenanth OC 15H 11O 0 G 300.00 5000.00 2030.00 1!Slavinskaya09,Richter2000
2.95619587E+01 4.24589619E-02-1.55841596E-05 2.54481062E-09-1.53124916E-13 2
2.56273028E+04-1.36219923E+02 1.33783643E-01 1.04067922E-01-5.92362501E-05 3
1.43179766E-08-9.91637313E-13 3.59458944E+04 2.35063505E+01 4
pyrene OC 16H 10O 0 G 200.00 6000.00 1!Slavinskaya09,Burcat 2007
0.29910014E+02 0.42668069E-01-0.15733834E-04 0.25851725E-08-0.15667980E-12 2
0.12786491E+05-0.14186953E+03-0.40420321E+01 0.91549657E-01 0.51443344E-04 3
-0.15276576E-06 0.73087530E-10 0.24094241E+05 0.43665312E+02 0.27145316E+05 4
nC3H7 C 3H 7O 0 G 0300.00 5000.00 1000.00 1
4.90850E+00 1.95492E-02 -6.09862E-06 9.08986E-10 -5.30994E-14 2
9.72711E+03 2.41566E-01 -9.97049E-01 4.22637E-02 -3.67683E-05 3
1.83985E-08 -3.66617E-12 1.08489E+04 2.87294E+01 4
o-methylbenzyl OC 8H 9O OG 0300.00 5000.00 1000.00 1!KINGAS
0.19563177E+02 0.21935524E-01-0.63449279E-05 0.89911217E-09-0.50900202E-13 2
0.11921492E+05-0.80102905E+02-0.21612432E+01 0.71680509E-01-0.45041892E-04 3
0.12837043E-07-0.13177945E-11 0.18941307E+05 0.35904976E+02 4
lC5H6 OC 5H 6O 0 G 0300.00 5000.00 1000.00 1
0.11761186E+02 0.15722809E-01-0.52564237E-05 0.82627116E-09-0.50267011E-13 2
0.25725818E+05-0.36669983E+02 0.60132211E+00 0.43948915E-01-0.28333196E-04 3

0.64557306E-08 0.31841822E-12 0.28983785E+05 0.21763247E+02 4
 methylindene OC 10H 100 OG 0300.00 5000.00 1000.00 1!Prof. Fournet
 1.71086085E+01 3.84373028E-02-1.51061240E-05 2.71490436E-09-1.83248686E-13 2
 6.59562283E+03-6.88187796E+01-5.69077766E+00 9.06507989E-02-4.13385689E-05 3
 -1.40869972E-08 1.33543495E-11 1.34969317E+04 5.17586359E+01 4
 fulvene 98 MARINOV&FC 6H 6 0 G 300.000 3000.000 1000.00 1!Mr.Pitz
 0.55099388E+01 0.33879936E-01-0.17737071E-04 0.44769284E-08-0.44127372E-12 2
 0.24921871E+05-0.67757489E+01-0.56096307E+01 0.73064757E-01-0.70326923E-04 3
 0.36580449E-07-0.80201931E-11 0.27468885E+05 0.48339178E+02 4
 SO OC 10H 100 0 G 0300.00 5000.00 1000.00 1!thergas
 0.17515572E+02 0.39169051E-01-0.14841164E-04 0.25519051E-08-0.16548222E-12 2
 0.27379234E+05-0.69436157E+02-0.71001720E+01 0.10770480E+00-0.74565884E-04 3
 0.16104806E-07 0.20384514E-11 0.33806332E+05 0.56861385E+02 4
 o-xylene OC 8H 100 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.17985743E+02 0.26968898E-01-0.88121678E-05 0.13625736E-08-0.81932447E-13 2
 -0.64873730E+04-0.72853989E+02-0.17060317E+01 0.70138752E-01-0.37771289E-04 3
 0.56106786E-08 0.11293696E-11-0.31772705E+02 0.32762829E+02 4
 phenyl(CH3)2 OC 8H 90 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.19200632E+02 0.21541221E-01-0.60772045E-05 0.84370538E-09-0.46977508E-13 2
 0.24025320E+05-0.77264038E+02-0.60923421E+00 0.62652625E-01-0.29779714E-04 3
 0.10032059E-08 0.21823782E-11 0.30694578E+05 0.29707020E+02 4
 HOC6H3(CH3)2 OC 8H 100 1G 0300.00 5000.00 1000.00 1!KINGAS
 0.29777200E+01 0.57097003E-01-0.23658878E-04 0.43309059E-08-0.29348648E-12 2
 -0.21476588E+05 0.13855827E+02-0.36083429E+01 0.89107245E-01-0.61163038E-04 3
 0.14350504E-07 0.16610515E-11-0.21290064E+05 0.42264072E+02 4
 !C3H5Y H 5C 3 0 OG 300.00 4000.00 1000.00 1
 !0.83240976E+01 0.99795023E-02-0.26202597E-05 0.34611722E-09-0.18670603E-13 2
 !0.15838413E+05-0.21291725E+02-0.71323484E+00 0.34044743E-01-0.28072202E-04 3
 !0.13918618E-07-0.31699231E-11 0.18564232E+05 0.26060329E+02 4
 OC6H3(CH3)2 OC 8H 90 1G 0300.00 5000.00 1000.00 1!KINGAS
 0.53072834E+01 0.48387561E-01-0.18405339E-04 0.31713454E-08-0.20584210E-12 2
 -0.40204531E+04 0.20877609E+01-0.38544981E+01 0.86276419E-01-0.60131446E-04 3
 0.14155940E-07 0.17449911E-11-0.30307119E+04 0.44200062E+02 4
 CH3C6H4CHO OC 8H 80 1G 0300.00 5000.00 1000.00 1!KINGAS
 0.34117519E+02 0.56146192E-02-0.10045563E-05 0.10052922E-09-0.45527724E-14 2
 -0.23880941E+05-0.16060309E+03-0.27612171E+01 0.73299579E-01-0.34734083E-04 3
 0.20300071E-08 0.98615126E-12-0.10282020E+05 0.42435173E+02 4
 CH3C6H4CO OC 8H 70 1G 0300.00 5000.00 1000.00 1!KINGAS
 0.32827263E+02 0.45028878E-02-0.59802443E-06 0.44885998E-10-0.15421790E-14 2
 -0.59170000E+04-0.15363544E+03-0.15736352E+01 0.60502756E-01-0.14559106E-04 3
 -0.12524174E-07 0.49236236E-11 0.72948896E+04 0.37936596E+02 4
 o-C6H4CHO OC 8H 70 1 G 0300.00 5000.00 1000.00 1!KINGAS
 0.34244980E+02 0.35322688E-02-0.38477933E-06 0.19851797E-10-0.19177666E-15 2
 -0.49546621E+04-0.16077888E+03-0.30528524E+01 0.73702835E-01-0.39264185E-04 3
 0.65173680E-08-0.49082781E-12 0.86914395E+04 0.44091377E+02 4
 !C6H4CHO OC 7H 50 1 G 0300.00 5000.00 1000.00 1!KINGAS
 !0.28160830E+02 0.30324757E-02-0.38583565E-06 0.30408790E-10-0.12342452E-14 2
 !0.00000000E+00-0.12728687E+03-0.21014626E+01 0.58027573E-01-0.24519395E-04 3
 !-0.32895986E-08 0.27161513E-11 0.00000000E+00 0.39256645E+02 4
 CH3C6H4CH2OOH OC 8H 100 2G 0300.00 5000.00 1000.00 1!KINGAS
 0.19242598E+02 0.32511316E-01-0.11088881E-04 0.17690666E-08-0.10879589E-12 2
 -0.17093045E+05-0.70666519E+02-0.36816618E+01 0.88307552E-01-0.53304513E-04 3

0.90592671E-08 0.19138287E-11-0.10222102E+05 0.50064514E+02 4
CH3C6H4CH2O OC 8H 9O 1G 0300.00 5000.00 1000.00 1!KINGAS
0.18246092E+02 0.27164159E-01-0.84199683E-05 0.12545508E-08-0.73559119E-13 2
0.99993750E+03-0.70436073E+02-0.63662777E+01 0.87856986E-01-0.59508522E-04 3
0.17500103E-07-0.13271282E-11 0.84847363E+04 0.59329815E+02 4
CH3HOC6H3CH2 OC 8H 9O 1G 0300.00 5000.00 1000.00 1!KINGAS
0.58374796E+01 0.49062986E-01-0.18995732E-04 0.33142904E-08-0.21703491E-12 2
-0.34346816E+04-0.96413422E+00-0.40454440E+01 0.90524793E-01-0.68138215E-04 3
0.21284459E-07-0.68326312E-12-0.23011333E+04 0.44540611E+02 4
!o-OC6H4CHO OC 8H 7O 2 G 0300.00 5000.00 1000.00 1!KINGAS
!0.35511753E+02 0.46037291E-02-0.64719376E-06 0.57258059E-10-0.25973054E-14 2
!-0.15752984E+05-0.16482683E+03-0.49355297E+01 0.85081816E-01-0.51337960E-04 3
!0.12065501E-07-0.13514468E-11-0.13801123E+04 0.55774872E+02 4
!C6H5CHO-1 OC 8H 6O 2 G 0300.00 5000.00 1000.00 1
!0.27822605E+02 0.62637692E-02-0.14661670E-05 0.18006827E-09-0.93566283E-14 2
!-0.15845393E+05-0.12738686E+03-0.34431257E+01 0.66832952E-01-0.34990375E-04 3
!0.32432945E-08 0.11444751E-11-0.46860913E+04 0.43472546E+02 4
CH3HOC6H3CH2OOC OC 8H 9O 3G 0300.00 5000.00 1000.00 1!KINGAS
0.17258772E+02 0.36663685E-01-0.12488573E-04 0.19889717E-08-0.12208972E-12 2
-0.19589164E+05-0.57327255E+02-0.38936484E+01 0.98721966E-01-0.71025264E-04 3
0.19093131E-07 0.36934079E-12-0.14327979E+05 0.50174309E+02 4
CH3HOC6H3CH2O OC 8H 9O 2G 0300.00 5000.00 1000.00 1!KINGAS
0.14892568E+02 0.36516245E-01-0.12552139E-04 0.20145297E-08-0.12445910E-12 2
-0.18746570E+05-0.47999687E+02-0.54567342E+01 0.95836043E-01-0.70005844E-04 3
0.21402876E-07-0.10586779E-11-0.13566174E+05 0.55746147E+02 4
CH3C6H4OH# OC 7H 7O 1G 0300.00 5000.00 1000.00 1!KINGAS
0.66537037E+01 0.36933094E-01-0.13681452E-04 0.23139142E-08-0.14823853E-12 2
0.12006594E+05-0.57214355E+01-0.25121901E+01 0.68031728E-01-0.41433053E-04 3
0.43510440E-08 0.35887847E-11 0.13617020E+05 0.38758183E+02 4
CH3OHC6H3CHO OC 8H 8O 2G 0300.00 5000.00 1000.00 1!KINGAS
0.32458767E+02 0.11561134E-01-0.29993710E-05 0.39136680E-09-0.20858318E-13 2
-0.44221500E+05-0.14739209E+03-0.17718489E+01 0.80726810E-01-0.43921573E-04 3
0.46528523E-08 0.16946174E-11-0.32341455E+05 0.38510689E+02 4
CH3C6H3OHCO OC 8H 7O 2G 0300.00 5000.00 1000.00 1!KINGAS
0.31635967E+02 0.95191598E-02-0.20342666E-05 0.23005084E-09-0.11129212E-13 2
-0.26421076E+05-0.14296658E+03-0.53421551E+00 0.67586049E-01-0.22928025E-04 3
-0.10711355E-07 0.59166179E-11-0.14769948E+05 0.33802353E+02 4
CH3C6H4CH2OH OC 8H 10O 1G 0300.00 5000.00 1000.00 1!KINGAS
0.16857079E+02 0.32344311E-01-0.11120477E-04 0.17840788E-08-0.11014143E-12 2
-0.24402434E+05-0.61932770E+02-0.49233394E+01 0.83134867E-01-0.47137404E-04 3
0.65180830E-08 0.21309319E-11-0.17643369E+05 0.53600662E+02 4
CH3C6H4CHOH OC 8H 9O 1G 0300.00 5000.00 1000.00 1!KINGAS
0.17559624E+02 0.27615020E-01-0.85476622E-05 0.12725067E-08-0.74580119E-13 2
-0.77037871E+04-0.64790482E+02-0.36830685E+01 0.76783471E-01-0.45183031E-04 3
0.96540660E-08 0.25431190E-12-0.99470038E+03 0.48222000E+02 4
CH3C6H4CH2CH3 OC 9H 12O 0G 0300.00 5000.00 1000.00 1!KINGAS
0.11256774E+02 0.47719818E-01-0.17962011E-04 0.30729026E-08-0.19848888E-12 2
-0.62495781E+04-0.32471664E+02-0.40742207E+01 0.91754116E-01-0.56702851E-04 3
0.11016761E-07 0.18377179E-11-0.24153237E+04 0.45610214E+02 4
CH3C6H4CHCH3 OC 9H 11O 0G 0300.00 5000.00 1000.00 1!KINGAS
0.12536176E+02 0.41745074E-01-0.14523367E-04 0.23501521E-08-0.14599235E-12 2
0.10266457E+05-0.38537170E+02-0.26020954E+01 0.83781444E-01-0.50582603E-04 3

0.97767208E-08 0.15654161E-11 0.14207361E+05 0.39124176E+02 4
 CH3styrene OC 9H 100 OG 0300.00 5000.00 1000.00 1!KINGAS
 -0.64905424E+01 0.74284628E-01-0.32960350E-04 0.63375678E-08-0.44518054E-12 2
 0.15234238E+05 0.65877571E+02-0.45196443E+01 0.92458449E-01-0.64155669E-04 3
 0.13829308E-07 0.29229772E-11 0.12028299E+05 0.46347641E+02 4
 o-bibenzyl OC 16H 180 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.29261724E+02 0.43097604E-01-0.14416902E-04 0.22686193E-08-0.13819160E-12 2
 0.29229766E+04-0.12956789E+03-0.79756641E+01 0.13282672E+00-0.83534906E-04 3
 0.17292775E-07 0.14303181E-11 0.14265402E+05 0.67088593E+02 4
 o-C14H13# OC 16H 170 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.30103733E+02 0.37990488E-01-0.11680387E-04 0.17287739E-08-0.10081936E-12 2
 0.19640207E+05-0.13268613E+03-0.74009504E+01 0.13168226E+00-0.92911367E-04 3
 0.29882159E-07-0.32315780E-11 0.30963801E+05 0.64709000E+02 4
 o-stilbene OC 16H 160 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.27049076E+02 0.42484868E-01-0.14866303E-04 0.24158795E-08-0.15054021E-12 2
 0.16342727E+05-0.11852699E+03-0.79815249E+01 0.13243322E+00-0.88932597E-04 3
 0.19873895E-07 0.15022144E-11 0.26392855E+05 0.64308105E+02 4
 benzocyclobut OC 8H 80 0 G 0300.00 5000.00 1000.00 1!KINGAS
 0.18383469E+02 0.22903126E-01-0.77421710E-05 0.12267607E-08-0.75054892E-13 2
 -0.15148281E+04-0.91357630E+02-0.29781268E+01 0.72204180E-01-0.42937296E-04 3
 0.68763590E-08 0.15090164E-11 0.51987344E+04 0.22200710E+02 4
 benzocyclobutyl OC 8H 70 0 G 0300.00 5000.00 1000.00 1!KINGAS
 0.20082308E+02 0.16943637E-01-0.47728067E-05 0.66350708E-09-0.37069448E-13 2
 0.14726205E+05-0.98979874E+02-0.19849489E+01 0.67901991E-01-0.42128067E-04 3
 0.82937710E-08 0.78630727E-12 0.21693797E+05 0.18425339E+02 4
 styryl THERGAS OC 8H 70 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.16176041E+02 0.21759402E-01-0.66688217E-05 0.98414743E-09-0.57243313E-13 2
 0.41049367E+05-0.59604996E+02-0.23101082E+01 0.66132776E-01-0.37655747E-04 3
 0.30604628E-08 0.29490531E-11 0.46557465E+05 0.37769215E+02 4
 !C2H2T C 2H 20 0 G 0300.00 5000.00 1000.00 1
 !3.00338E+00 7.58476E-03 -3.11008E-06 5.64312E-10 -3.79570E-14 2
 !2.62468E+04 5.29247E+00 2.54593E+00 1.14007E-02 -7.07123E-06 3
 !-6.00363E-10 1.71894E-12 2.60564E+04 6.56609E+00 4
 !C10H9 OC 10H 90 OG 0300.00 5000.00 1000.00 1!KINGAS
 !0.24414486E+02 0.23370475E-01-0.68964450E-05 0.98890962E-09-0.56302629E-13 2
 !0.19486688E+05-0.11926744E+03-0.23974934E+01 0.87768093E-01-0.56264824E-04 3
 !0.11641881E-07 0.10566989E-11 0.27670141E+05 0.22400475E+02 4
 !C10H10 OC 10H 100 OG 0300.00 5000.00 1000.00 1!KINGAS
 !0.19567667E+02 0.33812221E-01-0.11952324E-04 0.19566262E-08-0.12256583E-12 2
 !0.70208867E+04-0.93697594E+02-0.43665595E+01 0.89807026E-01-0.52336651E-04 3
 !0.81909759E-08 0.19331123E-11 0.14449433E+05 0.33239506E+02 4
 p-xylene OC 8H 100 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.17088512E+02 0.28108800E-01-0.92846949E-05 0.14457705E-08-0.87311004E-13 2
 -0.64339473E+04-0.68194397E+02-0.31023767E+01 0.72735257E-01-0.39950613E-04 3
 0.66947181E-08 0.86978851E-12 0.16202747E+03 0.39996910E+02 4
 p-methylbenzyl OC 8H 90 OG 0300.00 5000.00 1000.00 1!KINGAS
 0.19086742E+02 0.22677740E-01-0.66649313E-05 0.95677699E-09-0.54727249E-13 2
 0.11944541E+05-0.78811882E+02-0.31683695E+01 0.76185107E-01-0.53166041E-04 3
 0.19404270E-07-0.32588472E-11 0.18975293E+05 0.39316032E+02 4
 C6H5CHp-2 OC 8H 70 1 G 0300.00 5000.00 1000.00 1
 0.27822605E+02 0.62637692E-02-0.14661670E-05 0.18006827E-09-0.93566283E-14 2
 -0.15845393E+05-0.12738686E+03-0.34431257E+01 0.66832952E-01-0.34990375E-04 3

0.32432945E-08 0.11444751E-11-0.46860913E+04 0.43472546E+02 4
 p-etC6H4 0C 9H 11O 0 G 0300.00 5000.00 1000.00 1!KINGAS
 0.29261724E+02 0.43097604E-01-0.14416902E-04 0.22686193E-08-0.13819160E-12 2
 0.29229766E+04-0.12956789E+03-0.79756641E+01 0.13282672E+00-0.83534906E-04 3
 0.17292775E-07 0.14303181E-11 0.14265402E+05 0.67088593E+02 4
 trimetbenz C 9H 12O 0G 0300.00 5000.00 1000.00 1!KINGAS
 0.57078276E+01 0.57825219E-01-0.23154053E-04 0.41373713E-08-0.27558928E-12 2
 -0.50093848E+04-0.44507904E+01-0.44493732E+01 0.94222344E-01-0.61137929E-04 3
 0.14483445E-07 0.10342963E-11-0.32379512E+04 0.44531319E+02 4
 p-xylylene 0C 8H 8O 0 G 0300.00 5000.00 1000.00 1!KINGAS CORRIGE
 0.20661358E+02 0.22550413E-01-0.80408590E-05 0.13246614E-08-0.83358444E-13 2
 0.17010347E+05-0.90276053E+02-0.35237708E+01 0.97227775E-01-0.80353369E-04 3
 0.22176920E-07 0.86388562E-12 0.22558691E+05 0.31067137E+02 4
 p-phtaldehyde 0C 8H 6O 2 G 0300.00 5000.00 1000.00 1
 0.27822605E+02 0.62637692E-02-0.14661670E-05 0.18006827E-09-0.93566283E-14 2
 -0.15845393E+05-0.12738686E+03-0.34431257E+01 0.66832952E-01-0.34990375E-04 3
 0.32432945E-08 0.11444751E-11-0.46860913E+04 0.43472546E+02 4
 benzylCH2OH 0C 8H 9O 1G 0300.00 5000.00 1000.00 1!KINGAS
 0.18663233E+02 0.26807522E-01-0.83071782E-05 0.12389839E-08-0.72778155E-13 2
 -0.60488594E+04-0.71199005E+02-0.54818187E+01 0.85398257E-01-0.56156608E-04 3
 0.15503588E-07-0.94288954E-12 0.13585059E+04 0.56385750E+02 4
 HObenzylCH2OH 0C 8H 10O 2G 0300.00 5000.00 1000.00 1!KINGAS
 0.18497044E+02 0.33141427E-01-0.11299787E-04 0.18014045E-08-0.11068051E-12 2
 -0.42236039E+05-0.67202118E+02-0.58865099E+01 0.91805778E-01-0.55241926E-04 3
 0.94331361E-08 0.18873679E-11-0.34844824E+05 0.61496803E+02 4
 aC3H3 allenyl 0C 3H 3O 0G 200.00 6000.00 1000.00 1!Burkat
 6.32980309E+00 8.34146204E-03-2.93568490E-06 4.67354593E-10-2.77041642E-14 2
 3.92839304E+04-8.87103848E+00 1.31886167E+00 2.13679507E-02-1.10465018E-05 3
 -3.52008462E-09 4.05500469E-12 4.06655512E+04 1.70807075E+01 4.19058711E+04 4
 END

REACTIONS

!*****!

!especes excitees!

R1H+B10+M=OHE+M	6.0E14	0.0	6.94E3	!<HALL05>!
B4CH+O2=B2CO+OHE	4.0E13	0.0	0.0	!<HALL05>!
OHE+AR=R2OH+AR	5.2E10	0.5	0.0	!<HALL05>!
OHE+H2O=R2OH+H2O	8.6E12	0.5	0.0	!<HALL05>!
OHE+H2=R2OH+H2	1.5E12	0.5	0.0	!<HALL05>!
OHE+R1H=R2OH+R1H	1.5E12	0.5	0.0	!<HALL05>!
OHE+O2=R2OH+O2	1.5E12	0.5	0.0	!<HALL05>!
OHE+B10=R2OH+B10	1.5E12	0.5	0.0	!<HALL05>!
OHE+R2OH=R2OH+R2OH	1.5E12	0.5	0.0	!<HALL05>!
OHE=>R2OH			1.4E6 0.0 0.0	!<HALL05>!
OHE+CO2=R2OH+CO2	2.75E12	0.5	-968.	!<HALL05>!
OHE+B2CO=R2OH+B2CO	3.23E12	0.5	-787.	!<HALL05>!
OHE+CH4=R2OH+CH4	3.36E12	0.5	-635.	!<HALL05>!
R9C2H+B10=B2CO+CHE	6.2E12	0.0	0.0	!<HALL05>!
R9C2H+O2=CO2+CHE	2.17E10	0.0	0.0	!<HALL05>!
CHE+AR=B4CH+AR	4.0E10	0.5	0.0	!<HALL05>!

CHE+O2=B4CH+O2 2.48E6 2.14 0.0 !<HALL05>!
 CHE+H2O=B4CH+H2O 5.3E13 0.0 0.0 !<HALL05>!
 CHE+H2=B4CH+H2 1.47E14 0.0 1360. !<HALL05>!
 CHE+CO2=B4CH+CO2 2.41E-1 4.3 -1694. !<HALL05>!
 CHE+B2CO=B4CH+B2CO 2.44E12 0.5 0.0 !<HALL05>!
 CHE+CH4=B4CH+CH4 1.73E13 0.0 167. !<HALL05>!
 CHE=>B4CH 1.86E6 0.0 0.0 !<HALL05>!

!*****!
 ! 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>!
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 / 1.408E24 -1.8 0.0 /
TROE / 0.37 3315 61 /

CH4(+M)=>R4CH3+R1H(+M) 2.4E16 0. 105.0E3 !(-17)<BAULCH94>!
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/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>!
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/
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>!
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/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>!
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/
C2H4Z+M=R10C2H3V+R1H+M 7.40E17 0. 96.7E3 !(34,-34)<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/
!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
! 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 / 1.35E19 0.00 0.76E3 /
! TROE / 0.76 40 1025/
R11C2H5(+M)=C2H4Z+R1H(+M) 8.2E13 0. 40.0E3
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 / 3.40E17 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 2.3E17 0. 67.4E3 !(47,-47)<SCHULTZ85nIST>!
C2H6+R1H=R11C2H5+H2 1.4E9 1.5 7.4E3 !(48,-48)<BAULCH94>!
C2H6+B6CH2=R4CH3+R11C2H5 1.1E14 0. 0. !(49,-49)<TSAnG86>!
C2H6+R4CH3=R11C2H5+CH4 1.5E-7 6.0 5.8E3 !(50,-50)<BAULCH94>!
C2H6+R9C2H=C2H2+R11C2H5 3.6E12 0. 0. !(51,-51)<TSAnG86>!
C2H6+R10C2H3V=R11C2H5+C2H4Z 6.0E2 3.3 10.5E3 !(52,-52)<TSAnG86>!

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!*****!

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

!*****!

!***** REACTIONS DE B1O *****!

B1O+H2=R2OH+R1H 5.1E4 2.67 6.2E3 !(53,-53)<BAULCH94>!
B1O+B4CH=B2CO+R1H 3.9E13 0. 0. !(54,-54)<BAULCH94>!
B1O+B4CH=B3C+R2OH 1.5E13 0. 4.7E3 !(55,-55)<MUR86nIS>!
B1O+B6CH2=>B2CO+2R1H 1.5E13 0. 0. !(56) <TSAnG86>!
B1O+B6CH2=B2CO+H2 1.5E13 0. 0. !(57,-57) <TSAnG86>!
B1O+B5CH2=>B2CO+2R1H 7.2E13 0. 0. !(58) <BAULCH94>!
B1O+B5CH2=B2CO+H2 4.8E13 0. 0. !(59,-59)<BAULCH94>!
B1O+R4CH3=HCHO+R1H 8.4E13 0. 0. !(60,-60)<BAULCH94>!

B10+R4CH3=R7CH3O	8.0E15	-2.12	0.6E3	!(61,-61)<DEAn87nIS>!
B10+CH4=R4CH3+R2OH	7.2E8	1.56	8.4E3	!(62,-62)<BAULCH94>!
B10+R9C2H=B4CH+B2CO	1.0E13	0.	0.	!(63,-63)<DAGAUT91>!
B10+C2H2=B5CH2+B2CO	2.17E06	2.1	1.6E3	!(64,-64)<BAULCH LEEDS>!
B10+C2H2=R12CHCOZ+R1H	5.06E06	2.1	1.6E3	!(65,-65)<BAULCH LEEDS>!
R2OH+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=R2OH+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+R2OH	3.0E13	0.	0.	!(75,-75)<DAGAUT91>!
B10+C2H6=R11C2H5+R2OH	1.0E9	1.5	5.8E3	!(76,-76)<BAULCH94>!

!***** REACTIONS DE R2OH *****!

R1H+B10+M=R2OH+M	1.18E19	-1.0	0.0	
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/				
R1H+R2OH+M=H2O+M	5.53E+22	-2.0	0.0	
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/				
! N2/0.4/ HE/0.35/				
R2OH+H2=R1H+H2O	1.0E8	1.6	3.3E3	!(79,-79)<BAULCH94>!
R2OH+B3C=B2CO+R1H	5.0E13	0.	0.	!(80,-80)<RAnZI94>!
R2OH+B4CH=R5CHO+R1H	3.0E13	0.	0.	!(81,-81)<DAGAUT91>!
R2OH+B6CH2=HCHO+R1H	3.0E13	0.	0.	!(82,-82)<TSAnG86>!
R2OH+B5CH2=HCHO+R1H	1.8E13	0.	0.	!(83,-83)<TSAnG86>!
R2OH+R4CH3=B6CH2+H2O	7.2E13	0.	2.7E3	!(84,-84)<BAULCH94>!
R2OH+R4CH3(+M)=CH3OH(+M)	6.0E13	0.	0.	!(85,-85)<BAULCH94>!
LOW /1.4E44 -8.2 0./				
TROE /0.82 200. 1438./				
R2OH+R4CH3=HCHO+H2	3.2E12	-0.53	10.8E3	!(86,-86)<DAGAUT91>!
R2OH+R4CH3=R7CH3O+R1H	5.7E12	-0.23	13.9E3	!(87,-87)<DAGAUT91>!
R2OH+CH4=R4CH3+H2O	1.6E7	1.83	2.7E3	!(88,-88)<BAULCH94>!
!R2OH+R9C2H=C2H2+B10	1.8E13	0.	0.	!(89,-89)<TSAnG86>!
R2OH+R9C2H=B5CH2+B2CO	1.8E13	0.	0.	!(90,-90)<TSAnG86>!
R2OH+R9C2H=R12CHCOZ+R1H	2.0E13	0.	0.	!(91,-91)<DAGAUT91>!
R2OH+C2H2=R9C2H+H2O	3.385E+07	2.0	14000.0	!(92,-92)<KONNOV00>!
R2OH+C2H2=CH2COZ+R1H	1.100E+13	0.0	7170.0	!(93,-93)<KONNOV00>!
R2OH+C2H2=R4CH3+B2CO	4.8E-4	4.	-2.0E3	!(94,-94)<DAGAUT91>!
R2OH+R10C2H3V=C2H2+H2O	3.0E13	0.	0.	!(95,-95)<TSAnG86>!
R2OH+R10C2H3V=CH3CHO	3.0E13	0.	0.	!(96,-96)<TSAnG86>!
R2OH+C2H4Z=R10C2H3V+H2O	2.0E13	0.	5.9E3	!(97,-97)<BAULCH94>!
R2OH+C2H4Z=R4CH3+HCHO	2.0E12	0.	0.9E3	!(98,-98)<GLARBORG86>!
R2OH+R11C2H5=C2H4Z+H2O	2.4E13	0.	0.	!(99,-99)<TSAnG86>!
R2OH+R11C2H5=>R4CH3+R1H+HCHO	2.4E13	0.	0.	!(100) <TSAnG86>!
R2OH+C2H6=R11C2H5+H2O	7.2E6	2.	0.9E3	!(101,-101)<BAULCH94>!
R2OH+R2OH=H2O+B10	1.5E9	1.14	0.1E3	!(102,-102)<BAULCH94>!

!***** REACTIONS DE H2O *****!

H2O+B4CH=R6CH2OH 5.7E12 0. -0.8E3 !(103,-103)<BAULCH94>!
H2O+B6CH2=CH3OH 1.8E13 0. 0. !(104,-104)<TSAng86>!

!REACTIOns DE B2CO!

B2CO+R4CH3(+M)=R14CH3CO(+M) 5.0E11 0. 6.9E3 !(105,-105)<BAULCH94>!
LOW /1.1E14 0. 3.8E3/
TROE /0.5 1.0 1.0E8/
B2CO+B10+M=CO2+M 1.54E15 0.0 3.0E3 !(106,-106)<TSAng86>!
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/
B2CO+R2OH=CO2+R1H 6.3E6 1.5 -0.5E3 !(107,-107)<BAULCH94>!

!REACTIOns DE R5CHO!

R5CHO+M=R1H+B2CO+M 1.9E17 -1. 17.0E3 !(108,-108)<WAnG97>!
H2/2.0/ B2CO/1.5/ CO2/2.0/ H2O/6.0/
R5CHO+R1H=H2+B2CO 9.0E13 0. 0. !(109,-109)<BAULCH94>!
R5CHO+R1H=B10+B5CH2 4.0E13 0. 102.5E3 !(110,-110)<TSUBOI81nIST>!
R5CHO+B6CH2=R4CH3+B2CO 1.8E13 0. 0. !(111,-111)<TSAng86>!
R5CHO+B5CH2=R4CH3+B2CO 1.8E13 0. 0. !(112,-112)<TSAng86>!
R5CHO+R4CH3=CH4+B2CO 1.2E14 0. 0. !(113,-113)<TSAng86>!
R5CHO+R4CH3=CH3CHO 1.8E13 0. 0. !(114,-114)<TSAng86>!
R4CH3+HCHO=R5CHO+CH4 7.7E-8 6.1 1.97E3 !(115,-115)<BAULCH94>!
R5CHO+R9C2H=C2H2+B2CO 6.0E13 0. 0. !(116,-116)<TSAng86>!
R5CHO+R10C2H3V=C2H4Z+B2CO 9.0E13 0. 0. !(117,-117)<TSAng86>!
R10C2H3V+HCHO=R5CHO+C2H4Z 5.4E3 2.81 5.9E3 !(118,-118)<TSAng86>!
R5CHO+R11C2H5=C2H6+B2CO 1.2E14 0. 0. !(119,-119)<TSAng86>!
R11C2H5+HCHO=R5CHO+C2H6 5.57E3 2.81 5.86E3 !(120,-120)<TSAng86>!
R5CHO+B10=R1H+CO2 3.0E13 0. 0. !(121,-121)<BAULCH94>!
R5CHO+B10=R2OH+B2CO 3.0E13 0. 0. !(122,-122)<BAULCH94>!
R5CHO+R2OH=H2O+B2CO 1.1E14 0. 0. !(123,-123)<BAULCH94>!
R5CHO+R5CHO=HCHO+B2CO 3.0E13 0. 0. !(124,-124)<BAULCH94>!

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

HCHO+M=R5CHO+R1H+M 1.40E36 -5.54 96.8E3 !(125,-125)<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/
HCHO+M=H2+B2CO+M 3.26E36 -5.54 96.8E3 !(126,-126)<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/
HCHO+R1H=R5CHO+H2 1.3E8 1.62 2.1E3 !(127,-127)<BAULCH94>!
HCHO+B4CH=R13CH2CHO 9.6E13 0. -0.5E3 !(128,-128)<BAULCH94average>!
HCHO+B6CH2=R4CH3+R5CHO 1.2E12 0. 0. !(129,-129)<TSAng86>!
HCHO+B10=R5CHO+R2OH 4.1E11 0.57 2.7E3 !(130,-130)<BAULCH94>!
HCHO+R2OH=R5CHO+H2O 7.82E07 1.63 -1.06E3 !MF Vasudevan Int. J. Chem.
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!***** REACTIONS DE R7CH3O *****!

R7CH3O+M=HCHO+R1H+M 1.55E14 0.00 13.5E3
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/
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+B1O=HCHO+R2OH	1.8E12	0.	0.	!(143,-143)<BAULCH94>!
R7CH3O+R2OH=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>!
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/				
R6CH2OH+R1H=R4CH3+R2OH	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+B1O=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)<TSUBOI81nIST>!
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+R7CH3O	14.4	3.1	6.9E3	!(177,-177)<TSAnG87>!
CH3OH+R9C2H=C2H2+R6CH2OH	6.0E12	0.	0.	!(178,-178)<TSAnG87>!
CH3OH+R9C2H=C2H2+R7CH3O	1.2E12	0.	0.	!(179,-179)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R6CH2OH	31.9	3.2	7.2E3	!(180,-180)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R7CH3O	14.4	3.1	6.9E3	!(181,-181)<TSAnG87>!
CH3OH+B10=R6CH2OH+R2OH	3.4E13	0.	5.5E3	!(182,-
182)<GROTHER81nIST>!				
CH3OH+B10=R7CH3O+R2OH	1.0E13	0.	4.7E3	!(183,-183)<WARnATZ84>!
!modification des metatheses avec OH!				
!CH3OH+R2OH=R7CH3O+H2O	1.0E13	0.	1.7E3	!(184,-184)<WARnATZ84>!
CH3OH+R2OH=R6CH2OH+H2O	3.1E06	2.	-3.4E2	!(184a,-
184a)<Atkinson86>85%!				
CH3OH+R2OH=R7CH3O+H2O	5.4E05	2.	-3.4E2	!(184b,-
184b)<Atkinson86>15%!				
CH3OH+R7CH3O=CH3OH+R6CH2OH	3.0E11	0.	4.1E3	!(185,-185)<TSAnG87>!

!***** REACTIONS DE R12CHCO *****!

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

!***** REACTIONS DE CH2CO *****!

CH2COZ+M=B6CH2+B2CO+M	6.57E15	0.0	57.6E3	!(192,-192)<FRAnK86nIST>!
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/				
CH2COZ+M=R12CHCOZ+R1H+M	2.7E17	0.	87.0E3	!(193,-193)<FRAnK86nIST>!
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/				
CH2COZ+R1H=R4CH3+B2CO	1.8E13	0.	3.4E3	!(194,-194)<BAULCH94>!
CH2COZ+R1H=R12CHCOZ+H2	5.0E13	0.	8.0E3	!(195,-195)<DAGAUT91>!
CH2COZ+B5CH2=C2H4Z+B2CO	1.3E14	0.	0.	!(196,-196)<CAnOSA-MAS84nIST>!
CH2COZ+B10=B5CH2+CO2	1.8E12	0.	1.3E3	!(197,-197)<DAGAUT91>!
CH2COZ+B10=R12CHCOZ+R2OH	1.0E13	0.	8.0E3	!(198,-198)<DAGAUT91>!
CH2COZ+R2OH=R12CHCOZ+H2O	7.5E12	0.	2.0E3	!(199,-199)<DAGAUT91>!
!CH2COZ+R2OH=R5CHO+HCHO	2.8E13	0.	0.	!(200,-200)<VAnDOOREn77nIST>!
CH2COZ+R2OH=R4CH3+CO2	2.52E12	0.	0.	!(200a,-200a)<BAULCH LEEDS>!
CH2COZ+R2OH=R6CH2OH+B2CO	4.68E12	0.	0.	!(200b,-200b)<BAULCH
LEEDS>!				

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

R14CH3CO+R1H=R4CH3+R5CHO 9.6E13 0. 0. !(201,-201)<TSAnG86>!
R14CH3CO+B6CH2=R4CH3+CH2COZ 1.8E13 0. 0. !(202,-202)<TSAnG86>!
R14CH3CO+B5CH2=R4CH3+CH2COZ 1.8E13 0. 0. !(203,-203)<TSAnG86>!
R14CH3CO+B1O=R4CH3+CO2 9.6E12 0. 0. !(204,-204)<TSAnG86>!
R14CH3CO+R2OH=CH2COZ+H2O 1.2E13 0. 0. !(205,-205)<TSAnG86>!
R14CH3CO+R2OH=>R4CH3+B2CO+R2OH 3.0E13 0. 0. !(206)<TSAnG86>!
R14CH3CO+R5CHO=CH3CHO+B2CO 9.0E12 0. 0. !(207,-207)<TSAnG86>!
R14CH3CO+HCHO=CH3CHO+R5CHO 1.8E11 0. 12.9E3 !(208,-208)<TSAnG86>!
R14CH3CO+R7CH3O=CH3OH+CH2COZ 6.0E12 0. 0. !(209,-209)<TSAnG86>!
R14CH3CO+R7CH3O=HCHO+CH3CHO 6.0E12 0. 0. !(210,-210)<TSAnG86>!
R14CH3CO+CH3OH=CH3CHO+R6CH2OH 4.85E3 3. 12.3E3 !(211,-211)<TSAnG87>!
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 1.2E13 0. 0. !(212,-212)<TSAnG86>!

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

R13CH2CHO=R14CH3CO 1.0E13 0. 47.0E3 !(213,-213)<COLKET75nIST>!
R13CH2CHO=R1H+CH2COZ 1.6E13 0. 35.0E3 !(214,-214)<COLKET75nIST>!

!***** 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+B1O=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+B1O=R2OH+R13CH2CHO 1.9E12 0. 5.2E3 !(235,-235)<BOGAn78nIST>!
C2H4O#3+R2OH=H2O+R13CH2CHO 1.8E13 0. 3.6E3 !(236,-236)<BALDWIn84nIST*>!
C2H4O#3+R5CHO=HCHO+R13CH2CHO 3.7E12 0. 15.8E3 !(237,-237)<RAnZI94>!
C2H4O#3+R7CH3O=CH3OH+R13CH2CHO 1.3E12 0. 5.8E3 !(238,-238)<RAnZI94>!
C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO 8.4E11 0. 13.4E3 !(239,-239)<RAnZI94>!
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 *****!

R15C2H5O=HCHO+R4CH3 8.0E13 0. 21.5E3 !(242,-242)<BAULCH94>!

R15C2H5O=CH3CHO+R1H 2.0E14 0. 23.3E3 !(243,-243)<HEICKLEn88nIST>!

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

!Sous-mec repris de Marinov, IJCK 1999

C2H5OH(+M)=R11C2H5+R2OH(+M) 1.2E+23 -1.54 96.0E3 !<MARInOV99>

LOW /3.2E85 -18.81 114.9E3/

TROE /0.5 300.0 9.0E2 5.0E3/

CO2/3.0/ H2O/5.0/ B2CO/2.0/ H2/2.0/

C2H5OH(+M)=C2H4Z+H2O(+M) 2.8E+13 0.09 66.1E3 !<MARInOV99>

LOW /2.6E83 -18.85 86.5E3/

TROE /0.7 350.0 8.0E2 3.8E3/

H2O/5.0/

C2H5OH(+M)=CH3CHO+H2(+M) 7.2E+11 0.095 91.0E3 !<MARInOV99>

LOW /4.5E87 -19.42 115.6E3/

TROE /0.9 900.0 1.1E3 3.5E3/

H2O/5.0/

C2H5OH+R1H=H2+R15C2H5O 1.5E+07 1.6 3.04E+3 !<MARInOV99>!

C2H5OH+B10=R2OH+R15C2H5O 1.6E+07 2.0 4.45E+3 !<MARInOV99>!

C2H5OH+R2OH=H2O+R15C2H5O 7.5E+11 0.3 1.6E+3 !<MARInOV99>!

C2H5OH+R3OOH=H2O2+R15C2H5O 2.5E+12 0. 24.0E+3 !<MARInOV99>!

C2H5OH+R4CH3=CH4+R15C2H5O 1.4E+02 2.99 7.65E+3 !<MARInOV99>!

C2H5OH+R1H=H2+R2OH+C2H4Z 1.2E+07 1.8 5.1E+3 !<MARInOV99>!

C2H5OH+B10=R2OH+R2OH+C2H4Z 9.4E+07 1.7 5.46E+3 !<MARInOV99>!

C2H5OH+R2OH=H2O+R2OH+C2H4Z 1.7E+11 0.27 0.6E+3 !<MARInOV99>!

C2H5OH+R3OOH=H2O2+R2OH+C2H4Z 1.2E+04 2.55 15.7E+3 !<MARInOV99>!

C2H5OH+R4CH3=CH4+R2OH+C2H4Z 2.2E+02 3.18 9.6E+3 !<MARInOV99>!

C2H5OH+R1H=H2+CH3CHO+R1H 2.6E+07 1.65 2.8E+3 !<MARInOV99>!

C2H5OH+B10=R2OH+CH3CHO+R1H 1.9E+07 1.85 1.82E+3 !<MARInOV99>!

C2H5OH+R2OH=H2O+CH3CHO+R1H 4.6E+11 0.15 0. !<MARInOV99>!

C2H5OH+R3OOH=H2O2+CH3CHO+R1H 8.2E+03 2.55 10.7E+3 !<MARInOV99>!

C2H5OH+R4CH3=CH4+CH3CHO+R1H 7.3E+02 2.99 7.9E+3 !<MARInOV99>!

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

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

O2+R1H=R2OH+B10 9.8E13 0. 14.8E3 !(245,-245)<BAULCH94>!

!O2+R1H+M=R3OOH+M 2.10E18 -0.8 0.00 !(246,-246)<baseLeeds>!

! O2/0.4/ 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=R3OOH+H2O 6.90E15 0.0 -2.10E3 !(246,-246bis)<base Leeds>!

O2+R1H(+M)=R3OOH(+M) 4.52E13 0. 0. !(246,-246)<COBOS85>!

LOW /1.8E18 -0.8 0.00/

TROE /0.5 1.0 1.0E8/

O2/0.4/ 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)=R3OOH(+H2O) 1.63E14 0. 761. !(246b,-246b)<COBOS85>!

O2+R1H(+H2O)=R3OOH(+H2O) 4.52E13 0. 0. !(246b,-246b)<BAULCH94>!

LOW /6.9E15 0.0 -2080/

TROE /0.45 1.0 1.0E8/

O2+B3C=B2CO+B1O	1.2E14	0.	0.	!(247,-247)<RAnZI94>!
O2+B4CH=R5CHO+B1O	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>!
O2+B5CH2=B2CO+H2O	1.9E10	0.	-1.0E3	!(254,-254)<DAGAUT91>!
O2+B5CH2=>B2CO+R2OH+R1H	8.6E10	0.	-0.5E3	!(255)<DAGAUT91>!
O2+B5CH2=HCHO+B1O	1.0E14	0.	4.5E3	!(256,-256)<DAGAUT91>!
O2+R4CH3(+M)=R8CH300(+M)	7.8E8	1.2	0.	!(257,-257)<BAULCH94>!
	LOW /5.6E25	-3.3	0./	
	TROE /0.36	1.0	1.0E8/	
O2+R4CH3=R7CH30+B1O	1.3E14	0.	31.3E3	!(258,-258)<BAULCH94>!
!O2+R4CH3=R7CH30+B1O	1.6E13	0.	31.4E3	!(258,-258)<HWAnG&RABInOVITCH99>!
O2+R4CH3=HCHO+R2OH	3.0E30	-4.69	36.6E3	!(259,-259)<DAGAUT91>!
O2+CH4=R4CH3+R30OH	4.0E13	0.	56.7E3	!(260,-260)<BAULCH94>!
O2+R9C2H=B2CO+R5CHO	3.8E13	-0.16	0.	!(261,-261)<TIESEMA97/TSAng86>!
O2+R9C2H=R12CHCOZ+B1O	9.0E12	-0.16	0.	!(262,-262)<TIESEMA97/TSAng86>!
O2+C2H2=R9C2H+R30OH	1.2E13	0.	74.5E3	!(263,-263)<TSAng86>!
!O2+C2H2=R12CHCOZ+R2OH	2.0E8	1.5	30.1E3	!(264,-264)<DAGAUT91>!
O2+C2H2=R5CHO+R5CHO	7.0E7	1.8	30.6E3	!(264,-264)<BEnSO95>!
!O2+R10C2H3V=C2H2+R30OH	1.2E11	0.	0.	!(265,-265)<TSAng86>!
!O2+R10C2H3V=C2H2+R30OH	1.6E14	-0.83	2.5E3	!(265,-265)<WAnG97>!
!at 760 Torr				
!O2+R10C2H3V=HCHO+R5CHO	8.6E21	-2.97	3.3E3	!(266a,-266a)<WAnG97>!
!O2+R10C2H3V=B10+R13CH2CHO	1.2E13	-0.12	1.7E3	!(266b,-266b)<WAnG97>!
!at 20-90 Torr				
!O2+R10C2H3V=HCHO+R5CHO	1.6E21	-2.78	2.5E3	!(266a,-266a)<WAnG97>!
!O2+R10C2H3V=B10+R13CH2CHO	2.5E12	0.057	0.9E3	!(266b,-266b)<WAnG97>!
O2+R10C2H3V=C2H2+R30OH	1.34E6	1.61	-0.4E3	!(265,-265)<MEBEL nIST>!
O2+R10C2H3V=HCHO+R5CHO	4.5E16	-1.39	1.0E3	!(266a,-266a)<MEBEL nIST>!
O2+R10C2H3V=B10+R13CH2CHO	3.3E11	-0.29	10.	!(266b,-266b)<MEBEL nIST>!
O2+C2H4Z=R10C2H3V+R30OH	4.2E13	0.	57.4E3	!(267,-267)<TSAng86>!
O2+R11C2H5=R17C2H500	2.2E10	0.77	-0.6E3	!(268,-268)<WAGnER90>!
O2+R11C2H5=C2H4Z+R30OH	8.4E11	0.	3.9E3	!(269,-269)<TSAng86>!
O2+R11C2H5=R15C2H50+B1O	1.2E13	-0.2	27.9E3	!(270,-270)<BOZZELLI90nIST>!
O2+R11C2H5=CH3CHO+R2OH	6.0E10	0.	6.9E3	!(271,-271)<TSAng86>!
O2+C2H6=R11C2H5+R30OH	6.0E13	0.	51.7E3	!(272,-272)<BAULCH94>!
O2+R2OH=R30OH+B1O	2.2E13	0.	52.5E3	!(273,-273)<TSAng86>!
O2+B2CO=CO2+B1O	2.5E12	0.	47.7E3	!(274,-274)<TSAng86>!
!O2+R5CHO=B2CO+R30OH	5.1E13	0.	1.7E3	!(275,-275)<TSAng86>!
O2+R5CHO=B2CO+R30OH	7.6E12	0.	0.41E3	!(275,-275)<TIMOnEn88>!
O2+HCHO=R5CHO+R30OH	2.0E13	0.	38.8E3	!(276,-276)<TSAng86>!
O2+R7CH30=HCHO+R30OH	2.2E10	0.	1.7E3	!(277,-277)<BAULCH94>!
O2+R6CH2OH=HCHO+R30OH	1.2E12	0.	0.	!(278,-278)<TSAng87>!
O2+CH3OH=R6CH2OH+R30OH	2.0E13	0.	44.9E3	!(279,-279)<TSAng87>!

O2+R12CHCOZ=>B2CO+B2CO+R2OH 1.5E12 0. 2.5E3 !(280) <DAGAUT91>!
 !O2+CH2COZ=HCHO+CO2 1.0E8 0. 0. !(281,-281)<DAGAUT91>!bizarre
 O2+R14CH3CO=R18CH3COO 2.4E12 0. 0. !(282,-282)<COX90>!
 O2+R13CH2CHO=>HCHO+R2OH+B2CO 5.9E9 0. -1.4E3 !(283) <COX90>!
 O2+R13CH2CHO=CH2COZ+R3OOH 1.0E10 0. -1.4E3 !(284,-284)<COX90>!
 O2+CH3CHO=R14CH3CO+R3OOH 5.0E13 0. 36.4E3 !(285,-285)<COX90>!
 ! ajout demande par Laetitia le 25 Avril 95
 O2+CH3CHO=R13CH2CHO+R3OOH 1.0E13 0.5 46.0E3 !(285',-285)<Ranzi94>!
 O2+C2H4O#3=R3OOH+R13CH2CHO 5.0E13 0. 48.0E3 !(286,-286)<RAnZI94>!
 O2+R15C2H5O=CH3CHO+R3OOH 6.0E10 0. 1.7E3 !(287,-287)<BAULCH94>!

!***** REACTIONS DE R3OOH *****!

R3OOH+R1H=H2+O2 4.3E13 0. 1.4E3 !(288,-288)<BAULCH94>!
 R3OOH+R1H=2R2OH 1.7E14 0. 0.9E3 !(289,-289)<BAULCH94>!
 R3OOH+R1H=H2O+B1O 3.0E13 0. 1.7E3 !(290,-290)<BAULCH94>!
 R3OOH+B6CH2=HCHO+R2OH 3.0E13 0. 0. !(291,-291)<TSAng86>!
 R3OOH+B5CH2=HCHO+R2OH 1.8E13 0. 0. !(292,-292)<TSAng86>!
 R3OOH+R4CH3=R7CH3O+R2OH 1.8E13 0. 0. !(293,-293)<BAULCH94>!
 !R3OOH+R4CH3=R7CH3O+R2OH 4.0E13 0. 5.0E3 !(293,-293)<DAGAUT>
 R3OOH+CH4=R4CH3+H2O2 9.0E12 0. 24.6E3 !(294,-294)<BAULCH94>!
 R3OOH+R9C2H=R12CHCOZ+R2OH 1.8E13 0. 0. !(295,-295)<TSAng86>!
 R3OOH+C2H2=CH2COZ+R2OH 6.0E9 0. 8.0E3 !(296,-296)<TSAng86>!
 !incertitude au moins un facteur 10
 R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO 3.0E13 0. 0. !(297) <TSAng86>!
 R3OOH+C2H4Z=CH3CHO+R2OH 6.0E9 0. 7.9E3 !(298,-298)<TSAng86>!
 R3OOH+C2H4Z=C2H4O#3+R2OH 2.2E12 0. 17.2E3 !(299,-299)<BAULCH94>!
 R3OOH+R11C2H5=>R4CH3+HCHO+R2OH 2.4E13 0. 0. !(300) <TSAng86>!
 R3OOH+R11C2H5=C2H4Z+H2O2 3.0E11 0. 0. !(301,-301)<TSAng86>!
 R3OOH+C2H6=R11C2H5+H2O2 1.3E13 0. 20.4E3 !(302,-302)<BAULCH94>!
 R3OOH+R2OH=H2O+O2 2.9E13 0. -0.5E3 !(303,-303)<BAULCH94>!
 R3OOH+B2CO=CO2+R2OH 1.57E05 2.18 17.9E3 !MF Wang, J. Phys. Chem. A
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 R3OOH+R5CHO=>R2OH+R1H+CO2 3.0E13 0. 0. !(305) <TSAng86>!
 R3OOH+HCHO=R5CHO+H2O2 3.0E12 0. 13.0E3 !(306,-306)<BAULCH94>!
 R3OOH+R7CH3O=HCHO+H2O2 3.0E11 0. 0. !(307,-307)<TSAng86>!
 R3OOH+R6CH2OH=HCHO+H2O2 1.2E13 0. 0. !(308,-308)<TSAng87>!
 R3OOH+CH3OH=R6CH2OH+H2O2 9.6E10 0. 12.6E3 !(309,-309)<TSAng87>!
 R3OOH+R14CH3CO=>R4CH3+CO2+R2OH 3.0E13 0. 0. !(310)<TSAng86>!
 R3OOH+CH3CHO=R14CH3CO+H2O2 1.0E12 0. 10.0E3 !(311,-311)<CAVAnAGH90>!
 R3OOH+C2H4O#3=H2O2+R13CH2CHO 1.6E12 0. 15.0E3 !(312,-312)<RAnZI94>
 R3OOH+R3OOH=H2O2+O2 1.3E11 0. -1.63E3 !(313,-313)<BAULCH 94>!
 DUPLICATE
 R3OOH+R3OOH=H2O2+O2 4.2E14 0. 11.98E3 !(313,-313)<BAULCH 94>!
 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>!
HE/0.44/ 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+R3OOH 1.7E12 0. 3.7E3 !(315,-315)<BAULCH94>!
H2O2+R1H=H2O+R2OH 1.0E13 0. 3.6E3 !(316,-316)<BAULCH94>!
H2O2+B6CH2=R7CH3O+R2OH 3.0E13 0. 0. !(317,-317)<TSAng86>!
H2O2+R10C2H3V=C2H4Z+R3OOH 1.2E10 0. -0.6E3 !(318,-318)<TSAng86>!
H2O2+B10=R2OH+R3OOH 6.6E11 0. 4.0E3 !(319,-319)<BAULCH94>!
H2O2+R2OH=H2O+R3OOH 7.8E12 0. 1.3E3 !(320,-320)<BAULCH94>!

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

CO2+B5CH2=HCHO+B2CO 2.3E10 0. 0. !(321,-321)<TSAng86>!

!***** REACTIONS DE R8CH3OO *****!

R8CH3OO=HCHO+R2OH 1.5E13 0. 47.0E3 !(322,-322)<RAnZI94>!
R8CH3OO+R1H=R7CH3O+R2OH 9.6E13 0. 0. !(323,-323)<TSAng86>!
R8CH3OO+H2=CH3OOH+R1H 3.0E13 0. 26.0E3 !(324,-324)<TSAng86>!
R8CH3OO+B6CH2=HCHO+R7CH3O 1.8E13 0. 0. !(325,-325)<TSAng86>!
R8CH3OO+B5CH2=HCHO+R7CH3O 1.8E13 0. 0. !(326,-326)<TSAng86>!
R8CH3OO+R4CH3=R7CH3O+R7CH3O 5.0E12 0. -1.4E3 !(327,-327)<CAVAnAGH90>!
R8CH3OO+CH4=CH3OOH+R4CH3 1.8E11 0. 18.5E3 !(328,-328)<TSAng86>!
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ 2.4E13 0. 0. !(329,-329)<TSAng86>!
!R8CH3OO+C2H2=CH3OOH+R9C2H 5.6E11 0. 24.5E3 !(330,-330)<RAnZI94>! MF car i<<0
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 2.4E13 0. 0. !(331,-331)<TSAng86*>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3 1.1E15 0. 20.0E3 !(332,-
332)<nIKISHA81/MOSHKInA80nIST>!
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V 3.9E12 0. 24.5E3 !(333,-333)<RAnZI94>!
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O 2.4E13 0. 0. !(334,-334)<TSAng86>!
R8CH3OO+C2H6=CH3OOH+R11C2H5 2.9E11 0. 14.9E3 !(335,-335)<TSAng86>!
R8CH3OO+B10=R7CH3O+O2 3.6E13 0. 0. !(336,-336)<TSAng86>!
R8CH3OO+R2OH=CH3OH+O2 6.0E13 0. 0. !(337,-337)<TSAng86>!
R8CH3OO+R2OH=R7CH3O+R3OOH 3.0E12 0. 0. !(338,-338)<RAnZI94>!
R8CH3OO+B2CO=R7CH3O+CO2 1.0E14 0. 24.0E3 !(339,-339)<RAnZI94>!
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2 3.0E13 0. 0. !(340) <TSAng86>!
R8CH3OO+HCHO=CH3OOH+R5CHO 1.0E12 0. 12.1E3 !(341,-341)<CAVAnAGH90>!
R8CH3OO+R7CH3O=HCHO+CH3OOH 3.0E11 0. 0. !(342,-342)<TSAng86>!
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO 1.2E13 0. 0. !(343)<TSAng87>!
R8CH3OO+CH3OH=CH3OOH+R6CH2OH 1.8E12 0. 13.7E3 !(344,-344)<TSAng87>!
R8CH3OO+CH3OH=CH3OOH+R7CH3O 2.8E11 0. 18.8E3 !(345,-345)<RAnZI94>!
R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ 1.7E12 0. 27.0E3 !(346,-346)<RAnZI94>!
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O 2.4E13 0. 0. !(347,-347)<TSAng86>!
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO 1.0E12 0. 12.1E3 !(348,-348)<CAVAnAGH90>!
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO 1.7E12 0. 19.2E3 !(349,-349)<RAnZI94>!

R8CH300+C2H40#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>!

!***** REACTIOOnS DE CH300H *****!

CH300H=R7CH30+R2OH 6.0E14 0. 42.3E3 !(356,-356)<BAULCH94>!
CH300H+B10=R8CH300+R2OH 2.0E13 0. 4.8E3 !(357,-357)<BAULCH94average>!
CH300H+R2OH=H2O+R8CH300 1.8E12 0. -0.37E3 !(358,-358)<BAULCH94average>!
CH300H+R7CH30=>CH30H+R2OH+HCHO 1.5E11 0. 6.5E3 !(359)<RAnZI94>!

!***** REACTIOOnS 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+R2OH 5.6E12 0. 30.6E3 !(368,-368)<RAnZI94>!
R17C2H500+B2CO=CO2+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+R6CH2OH 2.8E12 0. 19.5E3 !(372,-372)<RAnZI94>!
R17C2H500+CH2COZ=C2H500H+R12CHCOZ 1.7E12 0. 24.4E3 !(373,-373)<RAnZI94>!
R17C2H500+CH3CHO=C2H500H+R14CH3CO 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=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+R2OH 1.5E11 0. 20.0E3 !(383,-383)<RAnZI94>!
R16C2H400H=R6CH2OH+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+R2OH 4.0E15 0. 42.9E3 !(386,-386)<BAULCH94>!
C2H500H+R1H=>CH3CHO+R2OH+H2 3.2E13 0. 7.7E3 !(387)<RAnZI94>!
C2H500H+R4CH3=>CH3CHO+R2OH+CH4 5.7E11 0. 8.7E3 !(388)<RAnZI94>!
C2H500H+R9C2H=>CH3CHO+R2OH+C2H2 6.0E11 0. 9.2E3 !(389)<RAnZI94>!
C2H500H+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12 0. 8.7E3 !(390)<RAnZI94>!
C2H500H+R11C2H5=>CH3CHO+R2OH+C2H6 3.4E11 0. 11.4E3 !(391)<RAnZI94>!
C2H500H+R2OH=>CH3CHO+R2OH+H2O 5.9E12 0. 0.9E3 !(392)<RAnZI94>!

C2H5OOH+R5CHO=>CH3CHO+R2OH+HCHO 1.8E12 0. 16.7E3 !(393)<RAnZI94>!
C2H5OOH+R7CH3O=>CH3CHO+R2OH+CH3OH 6.3E11 0. 5.5E3 !(394)<RAnZI94>!
C2H5OOH+R6CH2OH=>CH3CHO+R2OH+CH3OH 4.2E11 0. 13.6E3 !(395)<RAnZI94>!
C2H5OOH+R14CH3CO=>2CH3CHO+R2OH 2.0E12 0. 18.5E3 !(396)<RAnZI94>!
C2H5OOH+R13CH2CHO=>2CH3CHO+R2OH 3.4E11 0. 15.7E3 !(397)<RAnZI94>!
C2H5OOH+R3OOH=>CH3CHO+R2OH+H2O2 8.0E11 0. 16.2E3 !(398)<RAnZI94>!
C2H5OOH+R8CH3OO=>CH3CHO+R2OH+CH3OOH 1.1E12 0. 16.7E3 !(399)<RAnZI94>!
C2H5OOH+R17C2H5OO=>CH3CHO+R2OH+C2H5OOH 1.1E12 0. 16.7E3 !(400)<RAnZI94>!

!***** REACTIONS DE R18CH3COOO *****!

R18CH3COOO+C2H4O#3=CH3COOOH+R13CH2CHO 1.0E12 0. 9.3E3 !(401,-402)<RAnZI94>!
R18CH3COOO+R3OOH=CH3COOOH+O2 5.5E10 0. -2.6E3 !(402,-402)<COX90>!
R18CH3COOO+C2H5OOH=CH3COOOH+R17C2H5OO 5.0E11 0. 9.2E3 !(403,-403)<RAnZI94>!
R18CH3COOO+C2H5OOH=>CH3CHO+R2OH+CH3COOOH 5.0E11 0. 9.2E3 !(404)<RAnZI94>!
R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2 1.7E12 0. -1.0E3 !(405)<CAVAnAGH90>!

!***** REACTIONS DE CH3COOOH *****!

CH3COOOH=>R4CH3+CO2+R2OH 1.0E16 0. 40.0E3 !(406)<CAVAnAGH90>!

!*****

!*****

!*****!

! REACTIONS PRODUISANT DES C2+ RADICALAIRES !

!*****!

!MF car R20 n'intervient qu'ici

!R11C2H5+C2H4Z=>R20C4H9 1.1E11 0. 7.3E3 !(408)<BAULCH94>!

!*****!

! REACTIONS PRODUISANT DES C2+ MOLECULAIRES !

!*****!

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

!R9C2H+R9C2H=>C4H2 1.8E13 0. 0.!(24,-24)<TSAnG86>!

!***** REACTIONs DE C2H2 *****!

C2H2+B6CH2=aC3H4 1.7E14 0. 0.!(27,-27)<BAULCH94>!

C2H2+B5CH2=aC3H4 3.5E12 0. 0.!(28,-28)<TSAnG86>!

C2H2+R4CH3=>aC3H4+R1H 6.7E19 -2.08 31.6E3 !(29,-29)<DEAn87>!

!C2H2+R9C2H=>C4H2+R1H 9.0E13 0. 0.!(30,-30)<BAULCH94>!

C2H2+C2H2=>C4H4 5.5E12 0. 37.0E3 !(31,-31)<DURAn89>!

!***** REACTIONS DE C2H3 *****!

R10C2H3V+R4CH3=>C3H6Y 2.5E13 0. 0.!(37,-37)<TSAnG86>!

R10C2H3V+R9C2H=>C4H4 1.8E13 0. 0.!(38,-38)<TSAnG86>!

!R10C2H3V+C2H2=>C4H4+R1H 2.0E12 0. 5.0E3 !(40,-40)<FAHR89>!

!***** REACTIONS DE C2H4 *****!

!C2H4Z+B4CH=>aC3H4+R1H 1.3E14 0. -0.3E3 !(46,-46)<BAULCH94>! duplicate C3C6
!C2H4Z+B6CH2=>C3H6Y 9.6E13 0. 0. !(47,-47)<BAULCH94>! duplicate C3C6
!C2H4Z+B5CH2=>C3H6Y 3.2E12 0. 5.1E3 !(48,-48)<BAULCH94>!duplicate C3C6
!C2H4Z+R9C2H=>C4H4+R1H 1.2E13 0. 0. !(50,-50)<TSAnG86>!duplicate C3C6
!duplicate C2H4Z+R4CH3=>C3H6Y+R1H 6.6E11 0. 15.9E3 !<TSAnG86>!
!duplicate C2H4Z+R10C2H3V=>C4H6Z2+R1H 5.0E11 0. 7.3E3 !(51,-51)<TSAnG86>!

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

R11C2H5+R10C2H3V=>C4H8Y 1.5E13 0. 0. !(61,-61)<TSAnG86>!
R11C2H5+R11C2H5=>C4H10 1.1E13 0. 0. !(65,-65)<BAULCH94>!

!***** REACTIONS DE HCO *****!

R5CHO+R10C2H3V=>C2H3CHO 1.8E13 0. 0. !(138,-138)<TSAnG86>!
R5CHO+R11C2H5=>C2H5CHO 1.8E13 0. 0. !(141,-141)<TSAnG86>!

!***** REACTIONS DE CH3O *****!

!MF car CH3OCH3 n'intervient que dans cette réaction
!R7CH3O+R4CH3=CH3OCH3 1.2E13 0. 0. !(159,-159)<TSAnG86>!
!MF car CH3OOCH3 n'intervient que dans cette réaction
!R7CH3O+R7CH3O=>CH3OOCH3 1.8E12 0. 0. !(172,-172)<TSAnG86>!

!***** REACTIONS DE CH2OH *****!

!MF car C3H7OH n'intervient que dans cette réaction
!R6CH2OH+R11C2H5=C3H7OH 1.2E13 0. 0. !(189,-189)<TSAnG87>!

!***** REACTIONS DE CH3CO *****!

R14CH3CO+R4CH3=>C2H6CO 4.0E15 -0.8 0. !(231,-231)<TSAnG86>!
R14CH3CO+R11C2H5=>C3H8CO 3.1E14 -0.5 0. !(232,-232)<TSAnG86>!

!***** REACTIONS DE C3H8CO *****! suppression MF

!C3H8CO+R1H=>H2+CH2COZ+R11C2H5 2.7E+0007 2.000 5000.0 ! FCO 4057
!C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5 7.8E+0006 2.000 -765.0 ! FCO 4058
!C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5 1.2E+0012 0.000 15500.0 ! FCO 4059
!C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5 6.0E+0011 0.000 9600.0 ! FCO 4060
!C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5 6.0E+0011 0.000 9600.0 ! FCO 4061
!C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5 6.0E+0011 0.000 11000.0 ! FCO 4062

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

!C3H6Y+B10=CH3CHCO+2R1H 5.0E7 1.76 -1.22E3 !<TSAnG91>!
!CH3CHCO+R2OH=CH2CHCO+H2O 4.0E6 2.0 0.0 !<MARInOV>!
!CH3CHCO+B10=CH2CHCO+R2OH 7.2E12 0.0 2.0E3 !<MARInOV>!
!CH3CHCO+R1H=CH2CHCO+H2 2.0E5 2.5 2.5E3 !<MARInOV>!
!CH3CHCO+R1H=R11C2H5+B2CO 2.0E13 0.0 2.0E3 !<MARInOV>!
!CH3CHCO+B10=R4CH3+R5CHO+B2CO 3.0E7 2.0 0.0 !<MARInOV>!
!tC3H5+O2=CH3CHCO+R1H+B10 1.6E15 -0.78 3.1E3 !<MARInOV>!

!tC3H5+B10=CH3CHCO+R1H	1.0E14	0.0	0.0E3	!<MARInOV>!
!aC4H5+O2=CH3CHCO+R5CHO	4.2E10	0.0	2.5E3	!<SLAGLE92>!
C2H3CHO+R2OH=CH2CHCO+H2O	1.0E13	0.0	0.0	!<MARInOV>!
C2H3CHO+B10=CH2CHCO+R2OH	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+R3OOH	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+R3OOH=>C2H3CHO+R1H+R2OH	7.0E18	-2.0	0.0	!<TSAnG91>!
C3H5Y+O2=C2H3CHO+R2OH	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+R2OH=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+R2OH=C3H2+H2O	2.0E13	0.0	0.0	!<MILLER92>!
C3H3+R2OH=R10C2H3V+R5CHO	4.0E13	0.0	0.0	!<WAnG97>!
C2H2+R12CHCOZ=C3H3+B2CO	1.0E11	0.0	3.0E3	!<MILLER92>!
C3H3+O2=CH2COZ+R5CHO	3.0E10	0.0	2.9E3	!<MILLER92/SLAGUE88>!
C3H2+R1H=C3H3	1.0E14	0.0	0.0	!<est>!
C3H3+R3OOH=>R2OH+R9C2H+HCHO	1.0E15	-0.8	0.0	!<Heyberger>!
C3H3+C3H3=C6H6#	1.0E12	0.0	0.0	!<STEIn90>shocktube!
C3H3+C3H3=C6H5#+R1H	1.0E12	0.0	0.0	!<STEIn90>flame!

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

!pC3H4=>aC3H4	2.1E12	0.0	60.0E3	!<HIDAKA89>!
pC3H4+M=C3H3+R1H+M	4.7E18	0.0	80.0E3	!<HIDAKA89>!
C2H2+B5CH2=pC3H4	3.5E12	0.0	0.0	!<TSAnG86>!

pC3H4=R9C2H+R4CH3	4.2E15	0.0	125.0E3	!<KInGAS1500>!
pC3H4+O2=C3H3+R3OOH	2.1E12	0.0	40.8E3	!<est Ingham>!
pC3H4+R1H=C2H2+R4CH3	1.3E5	2.5	1.00E3	!<hidaka89>!

pC3H4+R1H(+M)=tC3H5(+M)	8.5E12	0.0	1.7E3	!<WAGnER72>!
LOW /5.6E25 -7.27 6.58E3/				!<Marinov97!
pC3H4+R1H(+M)=sC3H5(+M)	5.8E12	0.0	3.1E3	!<WAGnER72>!
LOW /3.8E25 -7.27 7.98E3/				!<estimated>!
pC3H4+R4CH3=C3H3+CH4	2.2E0	3.5	5.7E3	!<asTSAnG91>!
pC3H4+R1H=C3H3+H2	1.7E5	2.5	2.5E3	!<asTSAnG91>
pC3H4+R9C2H=C3H3+C2H2	3.6E12	0.0	0.0	!<asTSAnG91>!
pC3H4+R10C2H3V=C3H3+C2H4Z	2.2E0	3.5	4.7E3	!<asTSAnG91>!
pC3H4+R11C2H5=C3H3+C2H6	2.2E0	3.5	6.6E3	!<asTSAnG91>!
pC3H4+B10=R12CHCOZ+R4CH3	1.5E13	0.0	2.1E3	!<WARnATZ84>!
pC3H4+B10=R2OH+C3H3	3.4E4	2.16	4.8E3	!<<ADUSEI, G.Y, 1996>>!
pC3H4+R2OH=CH2COZ+R4CH3	4.3E11	0.0	-0.8E3	!<BOODAGHIANs87>!
pC3H4+R2OH=R1H+C2H3CHO	4.3E11	0.0	-0.8E3	!<asBOODAGHIANs87>!
pC3H4+R2OH=C3H3+H2O	3.1E6	2.0	-0.3E3	!<asTSAnG91>!
pC3H4+R3OOH=C2H4Z+B2CO+R2OH	6.0E9	0.0	8.0E3	!<as296<TSAnG86>!
pC3H4+R3OOH=C3H3+H2O2	9.6E3	2.6	13.9E3	!<asTSAnG91>!
pC3H4+R7CH3O=CH3OH+C3H3	2.0E12	0.0	4.0E3	!<Heyberger>!

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

aC3H4=pC3H4	2.5E12	0.0	59.0E3	!<HIDAKA89>!
aC3H4+M=C3H3+R1H+M	2.0E18	0.0	80.0E3	!<HIDAKA89>!
aC3H4+O2=C3H3+R3OOH	2.8E13	0.0	39.0E3	!<Estimation Ingham>!
aC3H4+R1H(+M)=C3H5Y(+M)			4.0E12 0.0 2.7E3	!<WAGnER72>!
LOW /5.6E33 -5.0 4.44E3/				!<Marinov97>
!				
aC3H4+R1H(+M)=tC3H5(+M)	8.5E12	0.0	2.0E3	!<WAGnER72>!
LOW /1.1E34 -5.0 4.44E3/				!<Marinov97!
C2H4Z+B4CH=aC3H4+R1H	1.3E14	0.0	-0.3E3	!<BAULCH94base>!
R10C2H3V+B5CH2=aC3H4+R1H	3.0E13	0.0	0.0	!<MILLER92>!
iC4H3+B5CH2=aC3H4+R9C2H	2.0E13	0.0	0.0	!<MILLER92>!
aC3H4+B10=R1H+B2CO+R10C2H3V	6.6E12	0.0	3.0E3	!<Aleksandrev nist>!
aC3H4+R2OH=CH2COZ+R4CH3	2.0E12	0.0	-0.2E3	!<LIU88>!
aC3H4+R2OH=HCHO+R10C2H3V	2.0E12	0.0	-0.2E3	!<LIU88>!
aC3H4+R1H=C3H3+H2	1.3E6	2.53	9.2E3	!<est.butatiene>!
aC3H4+B10=C3H3+R2OH	6.2E12	0.0	1.9E3	!<fromAleksandrev nist>!
!d'après leur vitesse de réaction total et d'addition !				
aC3H4+R2OH=C3H3+H2O	6.2E6	2.0	0.4E3	!<est.butadiene>!
aC3H4+R4CH3=C3H3+CH4	2.0E12	0.0	7.7E3	!<WU87>!
aC3H4+R9C2H=C3H3+C2H2	1.0E13	0.0	0.0	!<WU87>!
aC3H4+C3H5Y=C3H3+C3H6Y	2.0E12	0.0	7.7E3	!<DAGAUT92>
aC3H4+R7CH3O=CH3OH+C3H3			4.0E12 0.0 9.6E3	!<correlations a partir de Heyberger>!
aC3H4+R11C2H5=C2H6+C3H3		5.0E14	0.0 19.8E3	!<asbutadiene>!
aC3H4+R10C2H3V=C2H4Z+C3H3		5.0E14	0.0 19.8E3	!<asbutadiene>!
!aC3H4+R4CH3=C4H7T	5.7E10	0.0	6.8E3	!<Scherzer>!
!aC3H4+R4CH3=C4H7T	3.4E11	0.0	7.4E3	!<Tsang91x2>!
!aC3H4+R4CH3=iC4H7	1.6E11	0.0	5.0E3	!<Tsang73>!
!aC3H4+R4CH3=C4H7T			0.8E11 0.0 7.4E3	!<Tsang91x2/4>!

aC3H4+R4CH3=iC4H7 0.4E11 0.0 5.0E3 !<Tsang73/3>!

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

!aC3H4+C3H3=C6H6#+R1H 1.4E12 0.0 10.0E3 !<HIDAKA89>!

!***** REACTIONS DE cC3H4 ***** cyclopropene *****!

cC3H4=aC3H4 1.5E14 0.0 50.5E3 !<Karni>
cC3H4=pC3H4 7.1E13 0.0 47.8E3 !<Karni>
cC3H4+R1H=cC3H3+H2 5.4E4 2.5 -1.9E3 !<Heyberger>!
cC3H4+R2OH=cC3H3+H2O 3.0E6 2.0 -1.5E3 !<Heyberger>!
cC3H4+R2OH=C2H4Z+R5CHO 2.8E12 0.0 -1.0E3 !<Heyberger>!
cC3H3+R3OOH=R2OH+C2H2+R5CHO 1.0E15 -0.8 0.0 !<Heyberger>!
cC3H3+R4CH3=cC4H6 1.0E13 0.0 0.0 !<estimation>!
cC3H3+R1H=cC3H4 1.0E14 0.0 0.0 !<estimation>!

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

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

!réaction importante pour la formation de propène!

C3H5Y+R4CH3=aC3H4+CH4 3.0E12 -0.32 -0.1E3 !<TSAnG91>!
C3H5Y+R4CH3=C4H8Y 1.0E14 -0.32 -0.1E3 !<TSAnG91>!
C3H5Y+R2OH=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>!
!C3H5Y+R2OH=HCHO+C2H4Z 1.5E13 0.0 0.0 !<TSAnG91>!
!C3H5Y+R3OOH=R2OH+R5CHO+C2H4Z 5.0E12 0.0 0.0 !<asEXGAS>MODIF!!!!!!
!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 9.6E13 0.0 0.0 !<BAULCH94>!
C2H4Z+B5CH2=C3H6Y 3.2E12 0.0 5.1E3 !<BAULCH94>!
!duplicate R10C2H3V+R4CH3=C3H6Y 2.5E13 0.0 0.0 !<TSAnG86>!
C2H4Z+R4CH3=C3H6Y+R1H 6.6E11 0.0 15.9E3 !<TSAnG86>!
R11C2H5+B6CH2=C3H6Y+R1H 9.0E12 0.0 0.0 !<TSAnG86>!
C2H6+B4CH=C3H6Y+R1H 1.1E14 0.0 -0.3E3 !<BAULCH94>!
C3H6Y+R1H=sC3H5+H2 7.83E5 2.5 12.28E3 !<TSAnG92>!
C3H6Y+R1H=tC3H5+H2 3.9E5 2.5 5.82E3 !<TSAnG92>!
C3H6Y+R1H=C3H5Y+H2 1.7E5 2.5 2.5E3 !<TSAnG91>!
C3H6Y+R4CH3=C3H5Y+CH4 2.2E0 3.5 5.7E3 !<TSAnG91>!
C3H6Y+R4CH3=sC3H5+CH4 8.4E-1 3.5 11.7E3 !<TSAnG91>!
C3H6Y+R4CH3=tC3H5+CH4 1.3E0 3.5 12.9E3 !<TSAnG91>!
C3H6Y+R11C2H5=C3H5Y+C2H6 2.2E0 3.5 6.6E3 !<TSAnG91>!
C3H6Y+B10=>CH2COZ+R1H+R4CH3 1.2E+5 2.56 -1130.0 !<TSAnG91>! MF
C3H6Y+B10=C3H5Y+R2OH 1.7E11 0.7 5.9E3 !<TSAnG91>!
C3H6Y+R2OH=HCHO+R11C2H5 1.45E12 0.0 -0.9E3 !<TSAnG91>! MF
C3H6Y+R2OH=R4CH3+CH3CHO 1.45E12 0.0 -0.9E3
!<TSAnG91>! MF
C3H6Y+R2OH=C3H5Y+H2O 3.1E6 2.0 -0.3E3 !<TSAnG91>!
C3H6Y+R2OH=sC3H5+H2O 1.1E6 2.0 1.45E3 !<TSAnG91>!
C3H6Y+R2OH=tC3H5+H2O 2.1E6 2.0 2.8E3 !<TSAnG91>!
C3H6Y+O2=C3H5Y+R3OOH 1.9E12 0.0 39.0E3 !<WALKER93>!
C3H6Y+R3OOH=C3H5Y+H2O2 9.6E3 2.6 13.9E3 !<TSAnG91>!

C3H6Y+R9C2H=pC3H4+R10C2H3V 1.2E13 0.0 0.0 !TSANG 91 mehdi!

!***** 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+R2OH=C3H5Y+H2O 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
R19C3H7 = R1H+C3H6Y 3.000E+13 0.00 38000.00
iC3H7 = R1H+C3H6Y 6.000E+13 0.00 39000.00
R19C3H7 = iC3H7 1.960E+10 1.00 38600.00
!R19C3H7+O2 = R3OOH+C3H6Y 1.600E+12 0.00 5000.00
R19C3H7+O2 = R3OOH+C3H6Y 3.7e16 -1.63 3420 !2003DES/KLI4415-4427
iC3H7+O2 = R3OOH+C3H6Y 1.400E+12 0.00 5000.00

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

R11C2H5+R4CH3=C3H8 3.4E13 0. 0. !(59,-59)<BAULCH94>!
C3H8+O2=>R3OOH+iC3H7 1.4E+0013 0.000 50323.7 !BI 2 CN
C3H8+O2=>R3OOH+R19C3H7 4.2E+0013 0.000 53033.0 !BI 3 CN
B10+C3H8=>R2OH+iC3H7 2.6E+0013 0.000 5200.0 !ME 15 CW
B10+C3H8=>R2OH+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
C3H8+R2OH=>H2O+iC3H7 2.6E+0006 2.000 -765.0 !ME 19 CW
C3H8+R2OH=>H2O+R19C3H7 5.4E+0006 2.000 450.0 !ME 20 CW
C3H8+R3OOH=>H2O2+iC3H7 4.0E+0011 0.000 15500.0 !ME 21 CN
C3H8+R3OOH=>H2O2+R19C3H7 1.2E+0012 0.000 17000.0 !ME 22 CN
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
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
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

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!*****!

! REACTIONS DES ESPECES NON OXYGENES EN C4 !

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!***** 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 9.0E13 0.0 0.0 !BAULCH94!
!C4H2+R1H=C2H2+R9C2H 6.0E14 0.0 15.4E3 !<MEREDITH86>!
C4H2+R2OH=>R5CHO+C3H2 6.7E12 0.0 -0.4E3 !<LEEDS-website>!
C4H2+O2=R12CHCOZ+R12CHCOZ 9.6E12 0.0 31.1E3 !<HIDAKA02>!!!
C4H2+R9C2H=>C6H2+R1H 4.0E13 0.0 0.0 !<MEREDITH86>!
C6H2+R1H=>C4H2+R9C2H 9.3E14 0.0 15.1E3 !<MEREDITH86>!

!***** REACTIONS DE nC4H3 ***** (¥CH//CHC//CH) *****!

nC4H3(+M)=C4H2+R1H(+M) 1.0E14 0.0 36.0E3 !<MILLER92>!
LOW /1.0E14 0.0 30E3/
TROE / 1.0 1.0 1.0E8/
C3H3+B4CH=nC4H3+R1H 7.0E13 0.0 0.0 !<MILLER92>!
!C3H3+B4CH=nC4H3+R1H 5.0E13 0.0 0.0 !<MILLER92>!
R9C2H+R10C2H3V=nC4H3+R1H 1.8E13 0.0 0.0 !<TSAng86>!
nC4H3+R1H=iC4H3+R1H 2.4E11 0.79 2.41E3 !<WAnG97>20Torr!
nC4H3+R1H=C4H2+H2 0.6E13 0.0 0.0 !<0.5*la cst de la react(c2h3+h)>!
2C2H2=nC4H3+R1H 1.0E12 0.0 64.1E3 !<LEUnG95>!

nC4H3+R2OH=C4H2+H2O	1.5E13	0.0	0.0	!<0.5* la cst de la react(c2h3+oh)>!
!***				
!nC4H3+C2H2=C6H4#+R1H	1.64E9	0.73	12.2E3	!<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=C6H4#+R1H	3.0E-11	6.48	6.6E3	!<WESTMORELAnD89, p=101kPa>!
!***				
!nC4H3+C2H2=IC6H4+R1H	29.6	3.33	9.6E3	!<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=IC6H4+R1H	2.77E-7	5.59	6.0E3	!<WESTMORELAnD89, p=101kPa>!
!***				
!nC4H3+C2H2=IC6H5	1.73E11	-0.41	4.0E3	!<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=IC6H5	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//C#C///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 à la cst de la react(c2h3+h)>!
iC4H3+B10=CH2COZ+R9C2H	2.0E13	0.0	0.0	!<MILLER92>!
iC4H3+R2OH=C4H2+H2O	3.0E13	0.0	0.0	!<equiv à 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=>IC6H5+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	4.0E13	0.0	0.0	!<MEREDITH86>!
C2H2+iC4H3=>R9C2H+C4H4	3.0E13	0.0	27.9E3	!<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+nC4H3	5.0E11	0.0	16.3E3	!<MEREDITH86>!
nC4H3+C2H4Z=>R10C2H3V+C4H4	3.5E11	0.0	13.4E3	!<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+iC4H3	5.0E11	0.0	16.3E3	!<MEREDITH86>!
iC4H3+C2H4Z=>R10C2H3V+C4H4	1.3E11	0.0	24.1E3	!<MEREDITH86>!
C4H4+C2H2=C6H5#+R1H	1.0E09	0.0	30.02E3	!BENSON !MF
C4H4+R10C2H3V=C6H6#+R1H	1.9E12	0.0	2.5E3	!<LInSTEDT96>!
C4H4+B10=aC3H4+B2CO	3.0E13	0.0	1.8E3	!<LEUnG95>!
C4H4+B10=pC3H4+B2CO	2.7E13	0.0	1.8E3	!<MILLER>!
C4H4+R2OH=nC4H3+H2O	7.5E6	2.0	5.0E3	!<MILLER92>!

C4H4+R2OH=iC4H3+H2O	1.0E7	2.0	2.0E3	!<MILLER92>!
aC3H4+aC3H4=C2H4Z+C4H4	1.0E15	0.0	48.0E3	!<HIDAKA89>!

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

tC4H4+R2OH=iC4H3+H2O	2.0E7	2.0	2.0E3	!<Marinov>!
tC4H4+R1H=iC4H3+H2	3.0E7	2.0	6.0E3	!<Marinov>!

!***** REACTIONS DE nC4H5 ***** (¥CH//CHCH//CH2) *****

nC4H5(+M)=R1H+C4H4(+M)	1.0E14	0.0	37.0E3	!<MILLER92>!
LOW /1.00e+14 0.0 30000/				

nC4H5+R1H=C4H4+H2	1.5E13	0.0	0.0	!<WAnG97>!
nC4H5+R1H=iC4H5+R1H	1.0E14	0.0	0.0	!<MILLER92>!
nC4H5+R4CH3=C5H8	1.0E13	0.0	0.0	!<estimated>!

nC4H5=C2H2+R10C2H3V	1.0E14	0.0	43.9E3	!<HIDAKA96>!
!***				

!MF car lC6H6 n'intervient qu'ici

!nC4H5+C2H2=lC6H6+R1H	1.17E-15	7.84	2.0E3	!<WESTMORELAnD89, p=2.6kPa>!
!nC4H5+C2H2=lC6H6+R1H	3.47E-15	7.73	2.5E3	!<WESTMORELAnD89, p=101kPa>!
!***				

!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=lC6H7	8.74E12	-1.27	3.6E3	!<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=lC6H7	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=lC6H7+R1H	8.28E-28	11.89	5.0E3	!<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H7+R1H	3.55E-43	16.16	-0.2E3	!<WESTMORELAnD89, p=101kPa>!
!***				

!R10C2H3V+nC4H5=lC6H8	2.90E15	-0.78	1.0E3	!<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H8	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+R2OH=C4H4+H2O	2.5E12	0.0	0.0	!<WAnG97>!
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!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+R3OOH	5.19E15	-1.26	3.31e3	!MF as O2+C2H3=HCHO+CHO
<Marinov Combust. Flame114(1998)192 - 213>				

!***** REACTIONS DE iC4H5 ***** (CH2//CHC¥//CH2) *****stabilise par resonance
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 3.0E13 0.0 0.0 !<WAnG97>!
iC4H5+R4CH3=iC5H8 1.0E13 0.0 0.0 !<estimated> !
2R10C2H3V=iC4H5+R1H 1.5E30 -4.95 13.0E3 !<WAnG97>20Torr!
!***2R10C2H3V=iC4H5+R1H 1.2E22 -2.44 13.7E3 !<WAnG97>760Torr!
iC4H5+R2OH=C4H4+H2O 5.50E12 0.0 0.0 !<WAnG97>!
iC4H5+O2=HCHO+CH2CHCO 4.5E16 -1.39 1.0E3 !estimé par{O2+C2H3=HCHO+CHO}!
iC4H5+O2=C4H4+R3OOH 1.34E6 1.61 -400 !estimé par {O2+C2H3=C2H2+OOH}!

!***** REACTIONS DE C4H5-1s ***** (CH3/CH¥/C///CH) *****stabilise par resonance

!C4H5-1s=R1H+C4H4 3.0E13 0.0 45.0E3 !<HIDAKA96>!
C4H5-1s=R1H+C4H4 6.0E13 0.0 50.4E3 !add inverse!
! Les réactions suivantes sont deduities de celles de C3H3
C4H5-1s+R1H=C4H4+H2 2.0E13 0.0 0.0 !<MILLER92/BRAUn89>!
C4H5-1s+B10=R9C2H+CH3CHO 1.4E14 0.0 0.0 !<MILLER92/SLAGUE91>!
C4H5-1s+R2OH=C4H4+H2O 2.0E13 0.0 0.0 !<MILLER92>!
C4H5-1s+R2OH=R5CHO+sC3H5 4.0E13 0.0 0.0 !<WAnG97>!
C4H5-1s+O2=R5CHO+B2CO+C2H4Z 3.0E10 0.0 2.9E3 !<MILLER92/SLAGUE88>!
C4H5-1s+C4H5-1s=C8H10# 1.0E12 0.0 0.0 !<STEIn90>shocktube!

!***** REACTIONS DE C4H5-1p ***** (CH2¥/CH2/C///CH) *****

!C4H5-1p=R1H+C4H4 3.0E13 0.0 45.0E3 !<HIDAKA96>!
!C4H5-1p=R1H+C4H4 4.0E13 0.0 38.8E3 !<HIDAKA96>!
C4H5-1p=R9C2H+C2H4Z 2.0E14 0.0 57.0E3 !<HIDAKA96>!
C4H5-1p+O2=C4H4+R3OOH 1.6E12 0.0 5.0E3 !PAG00!
C4H5-1p=C4H5-1s 5.0E12 0.0 37.4E3 !PAG00!

!***** REACTIONS DE C4H5-2 ***** (CH3/C///C/CH2¥) *****stabilise par resonance

!C4H5-2=R1H+tC4H4 3.0E13 0.0 50.0E3 !<fromHIDAKA96+5>!
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 réactions suivantes sont deduities de celles de C3H3

C4H5-2+B10=C3H3+HCHO 1.4E14 0.0 0.0 !<MILLER92/SLAGUE91>!
C4H5-2+R2OH=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	6.3E10	0.0	7.49E3	! PERRIN 88 nist!
C4H6Z2+R4CH3=iC5H9	1.8E11	0.0	8.0E3	!Estimated*2!
!C4H6Z2+R4CH3=C5H9Y	6.31E10	0.0	7.49E3	! PERRIN 88 nist!
!C4H6Z2+R4CH3=iC5H9	9.64E10	0.0	8.0E3	!Estimated!
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+B2CO	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=iC6H8+R1H	1.0E10	1.05	14.0E3	!<WESTMORELAnD89,
p=2.6kPa>!				
R10C2H3V+C4H6Z2=iC6H8+R1H	2.48E-15	8.20	6.3E3	!<WESTMORELAnD89,
p=101kPa>!				
!***				
C4H6Z2+C2H2=C6H8#	2.3E12	0.0	35.0E3	!<WESTMORELAnD89>!
!***				
!MF car iC6H9 n'intervient qu'ici				
!R10C2H3V+C4H6Z2=iC6H9	5.48E28	-5.31	9.3E3	!<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=iC6H9	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+R2OH=nC4H5+H2O	6.2E6	2.0	3.4E3	!<WAnG97>!
C4H6Z2+R2OH=iC4H5+H2O	3.1E6	2.0	0.4E3	!<WAnG97>!
C4H6Z2+R2OH=C3H5Y+HCHO	2.8E12	0.0	-0.9E3	!<LInSTEDT96>!
C4H6Z2+R2OH=CH3CHO+R10C2H3V	5.6E12	0.0	-0.9E3	!<fromLInSTEDT96>!

C4H6Z2+O2=iC4H5+R3OOH	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+R2OH	1.7E11	0.7	5.9E3	!<asTSAnG91>!
C4H6-12+R2OH=iC4H5+H2O	3.1E6	2.0	-0.3E3	!<asTSAnG91>!
C4H6-12+R3OOH=iC4H5+H2O2	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	3.2E12	0.0	1.7E3	!<asWAGnER72>!
! Les réactions suivantes sont deduities 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=R2OH+C4H5-1s	8.8E10	0.7	3.2E3	!<EXGAS>!
C4H6-1+R2OH=H2O+C4H5-1s	3.0E6	2.0	-1.5E3	!<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1s	1.4E12	0.0	36.0E3	!<InGHAM95sec>!
C4H6-1+O2=>R3OOH+C4H5-1s	1.4E12	0.0	41.4E3	!<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s	4.2E12	0.0	49.5E3	!<DAGAUT90sec>!
C4H6-1+R3OOH=>H2O2+C4H5-1s	6.4E3	2.6	12.4E3	!<EXGAS>!
! Les réactions suivantes sont deduities 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=R2OH+C4H5-1p	5.1E13	0.0	7.8E3	!<EXGAS>!
C4H6-1+R2OH=>H2O+C4H5-1p	2.7E6	2.0	-0.4E3	!<EXGAS>!
C4H6-1+O2=>R3OOH+C4H5-1p	1.2E13	0.0	49.0E3	!<EXGAS>!

C4H6-1+R3OOH=>H2O2+C4H5-1p 6.0E11 0.0 17.0E3 !<EXGAS>!
 ! Les réactions d'addition suivantes sont deduities de celles de pC3H4
 C4H6-1+B1O=R12CHCOZ+R11C2H5 1.5E13 0.0 2.1E3 !<asWARnATZ84>!
 C4H6-1+R2OH=CH2COZ+R11C2H5 4.3E11 0.0 -0.8E3 !<asBOODAGHIANs87>!

!***** 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 2.0E14 0.0 87.3E3 !<HIDAKA96>!
 !C4H6-2+R1H=R4CH3+pC3H4 2.6E5 2.5 1.0E3 !<HIDAKA96>!
 C4H6-2+R1H=R4CH3+pC3H4 6.5E12 0.0 1.7E3 !<asWAGnER72>

! Les réactions 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+B1O=B2CO+R10C2H3V+R4CH3 1.5E13 0.0 2.1E3 !<asWARnATZ84>!
 C4H6-2+B1O=R2OH+C4H5-2 1.2E11 0.7 7.6E3 !<asTSAnG91*2>!
 C4H6-2+R2OH=B2CO+C2H4Z+R4CH3 4.3E11 0.0 -0.8E3 !<asBOODAGHIANs87>!
 C4H6-2+R2OH=C4H5-2+H2O 6.2E6 2.0 -0.3E3 !<asTSAnG91*2>!
 C4H6-2+O2=C4H5-2+R3OOH 4.2E12 0.0 44.0E3 !<InGHAM95*2>+4!
 C4H6-2+R3OOH=C4H5-2+H2O2 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)!*****stabilise 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+R3OOH=R2OH+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+R3OOH 3.6E12 0.0 38.2E3 !<Heyberger>!
C4H8Y+R1H=C4H7Y+H2 5.4E4 2.5 -1.9E3 !<Heyberger>!
C4H8Y+R2OH=>HCHO+R4CH3+C2H4Z 1.4E12 0.0 -1.0E3 !<Heyberger>!
C4H8Y+R2OH=R4CH3+C2H5CHO 1.4E12 0.0 -1.0E3 !<Heyberger>!
C4H8Y+R2OH=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+R2OH=H2O+B2CO+R11C2H5 4.0E12 0.0 0.5E3 !<Heyberger>!

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

iC4H8+R2OH=iC3H7+HCHO 1.4E12 0.0 -1040.0 !(idem RF)
iC4H8+R1H=>iC4H7+H2 3.5E5 2.5 2510 !(idem RF)
iC4H8+R2OH=>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+R3OOH=>R2OH+HCHO+tC3H5 1.0E15 -0.8 0.0 !<Heyberger>!

! REACTIONs DES ESPECES nOn OXYGENES En C5!

!*****Reactions of C5H7Y and iC5H7Y (CH2=CH-CH=CH-CH2•, CH2=C(CH2•)-CH=CH2)
!*****stabilises par resonance!

C5H7Y+R1H=C5H8 1.0E14 0.0 0.0 !Estimated!
iC5H7Y+R1H=iC5H8 1.0E14 0.0 0.0 !Estimated!
iC5H7Y=aC3H4+R10C2H3V 2.0E13 0.0 54.512E3 !MF DHr (thergas)=67.02 correlation
Baptiste 0.6*DH+14.3

!*****Reactions of iC5H8 and C5H8 (CH2=C(CH3)-CH-CH2, CH2=CH-CH=CH-CH3)!

C5H8+R1H=C5H7Y+H2 1.7E+05 2.50 2.5E3 !Estimated!
C5H8+R4CH3=C5H7Y+CH4 2.2E+00 3.50 5.67E3 !Estimated!
C5H8+R2OH=H2O+C5H7Y 3.0E6 2.0 -0.298E3 !Estimated!

iC5H8+R1H=iC5H7Y+H2 1.7E+05 2.50 2.5E3 !Estimated!
iC5H8+R4CH3=iC5H7Y+CH4 2.2E+00 3.50 5.67E3 !Estimated!
iC5H8+R2OH=H2O+iC5H7Y 3.0E6 2.0 -0.298E3 !Estimated!

!*****Reactions of C5H9Y (CH2=CH-CH•-CH2-CH3)

C5H9Y=R1H+C5H8 3.0E13 0.0 50.5E3 !Estimated HEYBERGER!
C5H9Y+R1H=H2+C5H8 1.8E13 0.0 0.0 !asTSANG 91!
C5H9Y+R1H=C5H10 2.0E13 0.0 0.0 ! Estimated TSANG !

!*****Reactions of iC5H9 (CH2•-CH(CH3)-CH=CH2)!

iC5H9=iC5H9Y 1.7E09 1 38.1E3 !Estimated
iC5H9=C3H6Y+R10C2H3V 2.0E13 0.0 35.5E3 !Estimated!
iC5H9=iC5H8+R1H 1.6E13 0.0 34.3E3 !Estimated!

!*****Reactions of iC5H9Y (CH3-C•(CH3)-CH=CH2)!

iC5H9Y=iC5H8+R1H	1.0E13	0.0	51.5E3	!Estimated
iC5H9Y+R1H=H2+iC5H8	1.8E13	0.0	0.0	!asTSANG 91!
iC5H9Y+R1H=iC5H10	2.0E13	0.0	0.0	!Estimated TSANG !
iC5H9Y+C3H5Y=iC5H8+C3H6Y	8.4E10	0.0	-0.3E3	!<asTSAnG91>!
iC5H9Y+iC5H9Y=iC5H8+iC5H10	8.4E10	0.0	-0.3E3	!<asTSAnG91>!

!*****Reactions of C5H10 and iC5H10 (CH2=CH-CH2-CH2-CH3, CH3-CH (CH3)-CH=CH2)

C5H10+R1H=C5H9Y+H2	5.4E4	2.5	-1.9E3	!Estimated!
C5H10+R4CH3=C5H9Y+CH4	1.0E11	0.0	7.3E3	!Estimated!
C5H10+R2OH=C5H9Y+H2O	3.0E6	2.0	-1.52E3	!Estimated!
iC5H10+R1H=iC5H9Y+H2	2.5E4	2.5	-2.8E3	!Estimated!
iC5H10+R4CH3=iC5H9Y+CH4	5.0E10	0.0	5.6E3	!Estimated!
iC5H10+R2OH=iC5H9Y+H2O	1.3E6	2.0	-2.6E3	!Estimated!

! REACTIO nS DES ESPECES nOn OXYGE nES En C6!

C6H4#+R1H=C6H5#	3.0E17	0.0	36.3E3	!WANG97!!
C6H8#+R1H=H2+C6H7#	1.1E05	2.5	-1900	!thèse de Dayma!
C6H8#+R2OH=H2O+C6H7#	6.0E6	2.0	-1520	!thèse de Dayma!
C6H8#=C6H6#+H2	1.28E28	-4.94	49.3E3	!ellis!

C6H10#=C6H9Z#+R1H 5.0E15 0.0 81.4E3 !<DEAn85>!

! ajout Roda : reaction de decomposition

!mf C6H9Z#=aC3H4+C3H5Y 2.0E13 0.0 33000 !HEYBERGER02 MF

C6H9Z#=>C2H4Z+nC4H5 1.3e+13 0.000 35900.0 !BH

C6H9Z#=R1H+C6H8# 3.0e+13 0.000 50500.0 !BH

!*****

!*****

!* MECHANISM FOR THE GAS PHASE OXIDATION OF CYCLOPENTENE *!

!* *!

!*****

!* PRIMARY MECHANISM OF THE OXIDATION OF CYCLOPENTENE *!

!*****

!*****

! Reactions moléculaires!

!*****

C5H8#=C5H6#+H2 2.2E13 0.0 60000 !Lewis74!

!*****

! Amorcages unimoléculaires!

!*****

C5H8-12=C5H8# 1.8E11 0.0 51.826E03 !Herzler et al 2001!

C5H8-12=C5H8 2.2E14 0.0 67.366E03 !Herzler et al 2001!

C5H8-12=C2H4Z+pC3H4 6.6E12 0.0 58.106E03 !Herzler et al 2001!

!C5H8-12=pentyne 1.6E13 0.0 64.187E03 !Herzler et al 2001!

!*****

C5H7#+R1H=C5H8#	1.0E14	0.0	0	! ALLARA ET SHAW)!
C5H7#Y+R1H=C5H8#	1.0E14	0.0	0	! ALLARA ET SHAW)!
C5H7#V+R1H=C5H8#	1.0E14	0.0	0	! ALLARA ET SHAW)!

!*****!

! Amorçages bimoléculaires!

!*****!

C5H8#+O2=C5H7#+R3OOH	1.4E13	0.0	47.6E3	!Ingham 94!
C5H8#+O2=C5H7#Y+R3OOH	2.8E12	0.0	35.6E3	!Ingham 94!
C5H8#+O2=C5H7#V+R3OOH	4.E12	0.0	60.07E3	!Ingham 94! MF Ea(thergas)

!*****!

!Réactions d'addition!

!*****!

!C5H9#=R1H+C5H8#	4.4E+14	0.104	37300.0	!SIRJEAN06
R1H+C5H8#=C5H9#	1.0E+14	0.0	3.26E3	!heyberger02*4!
!rev :	4.5E13	0.0	39000.0	
!améliore le propene et propyne!				
R2OH+C5H8#=>2C2H4Z+R5CHO	2.7E+12	0.0	-1.1E3	!heyberger02

!*****!

! Métathèses!

!*****!

!Avec H!

C5H8#+R1H=C5H7#+H2	9.0E06	2.0	5000	!BUDA05
C5H8#+R1H=C5H7#Y+H2	1.08E05	2.5	-1900	!HEYBERGER02
C5H8#+R1H=C5H7#V+H2	8.2E05	2.5	9790	!HEYBERGER02

!Avec OH!

C5H8#+R2OH=C5H7#+H2O	2.6E06	2.0	-770	!BUDA05
C5H8#+R2OH=C5H7#Y+H2O	6.0E06	2.0	-1520	!HEYBERGER02
C5H8#+R2OH=C5H7#V+H2O	2.2E06	2.0	1450	!HEYBERGER02

!Avec CH3!

C5H8#+R4CH3=C5H7#+CH4	2.0E11	0	9600	!BUDA05
C5H8#+R4CH3=C5H7#Y+CH4	2.0E11	0	7300	!HEYBERGER02
C5H8#+R4CH3=C5H7#V+CH4	1.96	3.5	11700	!HEYBERGER02

!Avec O!

C5H8#+B10=C5H7#+R2OH	2.6E13	0.0	5200	!BUDA05
C5H8#+B10=C5H7#Y+R2OH	1.7E11	0.7	3250	!HEYBERGER02
C5H8#+B10=C5H7#V+R2OH	1.2E11	0.7	7630	!HEYBERGER02

! Avec C2H5 !

C5H8#+R11C2H5=C5H7#+C2H6	2.0E11	0.0	11000	!HEYBERGER02
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C5H8#+R11C2H5=C5H7#Y+C2H6 8.8 3.5 4140 !HEYBERGER02

!*****!

!Isomérisations!

!*****!

C5H7#=C5H7#Y 2.3E11 1.0 44100 !estimated O'Neal +5kcal/mol!
C5H7#V=C5H7#Y 6.67E12 0.0 49500 !THESEHEYBERGER +5kcal/mol!
!+5kcal/mol a cause de la presence du cycle en C5!

!*****!

!Réactions par Béta-scission!

!*****!

! C5H7-1s(ch(./ch/ch2/ch//ch2), C5H7Y(ch2//ch/ch//ch/ch2(.)), C5H7-2t=ch2//ch/ch2/c(./ch2)!
! C5H7-3t(ch3/ch//c(./ch//ch2), C5H7-4t (ch3/c(./ch//ch2),
! C5H7-5p(ch2(./ch2/ch2/c//ch)! ! C5H7-12-5p(ch2(./ch2/ch//c//ch2)!

C5H7#=C5H7-1s 2.0E13 0.0 35500 !FROMHEYBERGER02

C5H7-1s=C2H2+C3H5Y 2.0E13 0.0 33000 !HEYBERGER02

C5H7#Y=C5H7Y 1.3E13 0.0 35900 !FROMHEYBERGER02

C5H7-1s=C5H7Y 3.4E13 0.0 34500 !THESEHEYBERGER

C5H7-2t=C5H7Y 1.3E13 0.0 44500 !THESEHEYBERGER

C5H7-3t=C5H7Y 5.0E13 0.0 37000 !THESEHEYBERGER

C5H7-4t=C5H7Y 2.0E13 0.0 47000 !THESEHEYBERGER

C5H7-2t=R10C2H3V+aC3H4 2.0E13 0.0 35500 !HEYBERGER02

C5H7-3t=R4CH3+C4H4 2.0E13 0.0 31500 !HEYBERGER02

C5H7-4t=R10C2H3V+pC3H4 2.0E13 0.0 38074 !HEYBERGER02 + MF DHr=39.624
correlation Baptiste E=0.6DHr+14.3

C5H7#V=C5H7-5p 2.0E13 0.0 33000 !FROMHEYBERGER02

C5H7#V=C5H7-12-5p 2.0E13 0.0 31000 !FROMHEYBERGER02

C5H7-5p=C2H4Z+C3H3 2.0E13 0.0 22500 !HEYBERGER02

C5H7-12-5p=C2H4Z+C3H3 2.0E13 0.0 35500 !HEYBERGER02

C5H7#=C5H6#+R1H 6.4E13 0.0 34800 !HEYBERGER02

C5H7#Y=C5H6#+R1H 3.0E13 0.0 50500 !HEYBERGER02!

! C5H9 (.)ch2/ch2/ch2/ch//ch2)

C5H9#=C5H9 2.0D+14 0.005 35600 !SIRJEAN05

C5H9=C3H5Y+C2H4Z 3.3D+13 0.000 22500 !EXGAS

C5H9=R1H+C5H8 3.0D+13 0.000 38000 !EXGAS

C5H9=C5H9Y 3.3E9 1.0 32350 !estimated O'Neal!

C5H9+O2=>C5H8+R3OOH 1.6D+12 0.000 5000 !EXGAS

!*****!

!OXYDATIONS DES RADICAUX!

!*****!

C5H7#+O2=C5H6#+R3OOH 5.2E11 0.0 2500 !TOUCHARD05

C5H7#Y+O2=C5H6#+R3OOH 1.58E12 0.0 15200 !TOUCHARD05

!*****!

!Terminaisons des radicaux allyliques!

!*****!

!C5H7#Y+R3OOH=R13CH2CHO+pC3H4+R2OH 1.0E15 -0.8 0.0 !HEYBERGER02
C5H7#Y+R3OOH=C2H4Z+CH2CHCO+R2OH 1.0E13 0.0 0.0 !asTSANG 91!
C5H7#Y+R1H=C5H6#+H2 1.8E13 0.0 0.0 !asTSANG 91!
C5H7#Y+R2OH=C5H6#+H2O 6.0E12 0.0 0.0 !asTSANG 91!
C5H7#Y+R4CH3=MCP 5.0E12 0.0 0.0 !KINGAS

!REACTIONS OF METHYLCYCLOPENTENE AND DERIVED RADICALS!

! MCP (c(#1)h2/ch2/ch//ch/ch(/ch3)/1) RMCP1 (c(#1)h(/)ch2/ch//ch/ch(/ch3)/1)
! RMCPY1 (c(#1)h2/ch(/)ch//ch/ch(/ch3)/1) RMCP2 (c(#1)h2/ch2/ch//ch/ch(/ch2(/)/1)
! RMCPY2 (c(#1)h2/ch2/ch//ch/c(/)ch3)/1)

MCP+R1H=RMCP1+H2 9.0E06 2.0 5000 !BUDA05
MCP+R1H=RMCPY1+H2 5.0E04 2.5 -1900 !HEYBERGER02
MCP+R1H=RMCP2+H2 2.9E7 2.0 7.7E3 !BUDA05
MCP+R1H=RMCPY2+H2 2.5E04 2.5 -2790 !HEYBERGER-these
MCP+R2OH=RMCP1+H2O 2.6E06 2.0 -770 !BUDA05
MCP+R2OH=RMCPY1+H2O 3.0E06 2.0 -1520 !HEYBERGER02
MCP+R2OH=RMCP2+H2O 2.7E6 2.0 0.45E3 !BUDA05
MCP+R2OH=RMCPY2+H2O 1.3E06 2.0 -2620 !HEYBERGER-these
!RMCP1=>C2H2+C4H7Y 2.0E13 0.0 31000 !HEYBERGER02
RMCP1=>C2H2+C4H7Y 2.0E13 0.0 40300 !HEYBERGER02
RMCP1=R4CH3+C5H6# 2.0E13 0.0 31000 !BUDA05
RMCP2=>C2H4Z+nC4H5 2.0E13 0.0 28700 !BUDA05
RMCP1+O2=MCPD+R3OOH 2.6E11 0.0 2500 !TOUCHARD05
RMCPY1+O2=MCPD+R3OOH 1.58E12 0.0 15200 !TOUCHARD05
RMCPY1+R1H=MCP 1.0E14 0.0 0.0 !ALLARA
RMCPY2+R1H=MCP 1.0E14 0.0 0.0 !ALLARA

!REACTIONS OF METHYLCYCLOPENTADIENE AND DERIVED RADICALS!

! MCPD (c(#1)h//ch/ch//ch/ch(/ch3)/1) RMCPDY (c(#1)h//ch/ch//ch/c(/)ch3)/1)
! RMCPD (c(#1)h//ch/ch//ch/ch(/ch2(/)/1)

C5H5#+R4CH3=MCPD 0.5E13 0.0 0.0 !KINGAS!
MCPD+R1H=C5H6#+R4CH3 1.00E13 0.0 1.3E3 !MARINOV98!
MCPD+R1H=RMCP1 2.6E13 0.0 3.2E3 !HEYBERGER02
MCPD+R1H=RMCPY1 2.6E13 0.0 3.2E3 !HEYBERGER02!
!MCPD+R1H=RMCPD+H2 1.0E14 0.0 10.0E3 !LIFSHITZ05
MCPD+R1H=RMCPD+H2 2.9E7 2.0 7.7E3 !BUDA05
MCPD+R2OH=RMCPD+H2O 2.7E6 2.0 0.45E3 !BUDA05
!MCPD+R1H=RMCPDY+H2 1.0E14 0.0 10.0E3 !LIFSHITZ05
MCPD+R1H=RMCPDY+H2 2.5E4 2.5 -2.7E3 !THESEHEYBERGER
MCPD+R2OH=RMCPDY+H2O 1.3E6 2.0 -2.7E3 !THESEHEYBERGER
RMCPDY=RMCPD 3.0E12 0.0 50.4E3 !LIFSHITZ05
RMCPD=C6H7# 1.4E13 0.0 17.4E3 !LIFSHITZ05
C6H6#+R1H=RMCPDY 2.39E27 -3.92 29.2E3 !MARINOV98!

!C6H7#=RMCPDY 5.00E12 0.0 38.1E3 !MARINOV98!
RMCPDY+R1H=MCPD 1.0E14 0.0 0.0 !ALLARA

MCPD+R4CH3=RMCPDY+CH4 0.9e-1 4.0 0e3 !estimated from C5H6+CH3!
MCPD+C6H5O#=RMCPDY+C6H5OH# 1.64e14 0.0 20934.21 !estimated from
C5H6+C6H5O!
MCPD+C5H5#=RMCPDY+C5H6# 1.58e11 0.0 8e3 !Pecullan_1997!

!REACTION GIVING TOLUENE!

!MFbenzyl=C5H5C2H2 3.2E15 0.0 42.9E3 !<Braun-Unkoff>-modif-fbl!
!MFC5H5C2H2=C5H5#+C2H2 2.0E13 0.0 33000 !HEYBERGER02-modif-fbl!
!benzyl=C5H5#+C2H2 1.0E16 0.0 70.0E3 !<Hippler*5/Colket94>-modif-fbl!
!rev : 2.77E12 0.0 3636.0
!MFC5H5#+C2H2=>benzyl 1.0E12 0.0 7000.0 !fitted-modif-fbl!

!*****!
!*****!
!* 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 initiation!

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 initiation!

C6H6#+O2=C6H5#+R3OOH 6.0E13 0.0 63.4E3 !<ALZUETA00>!

!***additions!

C6H6#+R1H=C6H7# 3.2E13 0.0 3.2E3 !<MEBEL97>!
C6H6#+B10=C6H5O#+R1H 2.8E13 0.0 4.91E3 !<EMDEE92>!
C6H6#+R2OH=C6H5OH#+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#+R2OH 2.0E13 0.0 14.7E3 !<LINDSTEDT94>!

!*modif Zhenyu*!

!C6H6#+R2OH=C6H5#+H2O 1.6E8 1.42 1.45E3 !<BAULCH92>!

C6H6#+R2OH=C6H5#+H2O 1.36E4 2.7 0.6196E3 !as
toluene+R2OH=C6H4CH3+H2O

!*modif Zhenyu*!
!C6H6#+R3OOH=C6H5#+H2O2 5.5E12 0.0 28.9E3 !<BAULCH94>!
C6H6#+R3OOH=C6H5#+H2O2 9.2E12 0.0 28.81E3 !as toluene+R3OOH=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!

C6H5#+C2H4Z=C6H6#+R10C2H3V 9.45e-3 4.47 4471 !Tokmakov 2004_nist!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=iC6H7 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#+R3OOH 7.9E11 0.0 9.9E3 !estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combiminations!
C6H7#+R1H=C6H8# 1.0E14 0.0 0.0 !estimated!
!***Disproportionnations!
C6H7#+R1H=C6H6#+H2 3.3E12 0.0 0.0 !<RISTORIO1>!
C6H7#+R2OH=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#=iC6H5 5.0E13 0.0 72.5E3 !<BRAUN89>!
!C6H5 = ch///c/ch//ch//ch(.)!
iC6H5=>2C2H2+R9C2H 2.0E13 0.0 51.0E3 !estimated!
!DH298 =44kcal/mol, Eadd=7 kcal/mol!
iC6H5=iC6H4+R1H 2.0E12 0.0 41.0E3 !estimated!
!C6H4 = 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#+B2CO 1.0E14 0.0 0.0 !<FRANK94>!

C6H5#+R2OH=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#+R3OOH=C6H5O#+R2OH 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>!

!***disproportionnations!

C6H5#+R2OH=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!

C6H5#+O2=>C6H5O2 1.86E13 -0.217 -0.711 ! da silva 2008

C6H5O2=>C6H5#+O2 6.36E19 -1.372 48.740 ! da silva 2008

C6H5O#+B10=>C6H5O2 2.81E13 -0.197 -1.935 ! da silva 2008

C6H5O2=>C6H5O#+B10 1.27E15 -0.246 38.536 ! da silva 2008

!MF

C6H5O2+R3OOH=C6H5OOH+O2 2.0E11 0.00 -1300

C6H5OOH=C6H5O#+R2OH 1.5E16 0.00 43000

!REACTIONS OF PHENOXY RADICALS!

!C6H5O#=bicycle 2.08E+13 0.182 51263.7 !CBS-QB3 1100 - 2000K k inf!

!C6H5O#=bicycle 1.09E+78 -18.464 91710.8 !CBS-QB3 1100 - 2000K k 2.5 bar!

C6H5O#=bicycle 6.17E+78 -18.794 90504.0 !CBS-QB3 1100 - 2000K k 1.2 bar!

!bicycle=C5H5#+B2CO 1.34E+13 -0.015 8531.0 !CBS-QB3 1100 - 2000K k inf!

!bicycle=C5H5#+B2CO 6.30E+23 -3.042 13478.3 !CBS-QB3 1100 - 2000K k 2.5 bar!

bicycle=C5H5#+B2CO 8.29E+20 -2.422 11112.0 !CBS-QB3 1100 - 2000K k 1.2 bar!

C5H5#+B10=C5H4O#+R1H 5.8E13 -0.02 0.02E3 !<ZHONG98>!
C5H5#+B10=>2C2H2+R5CHO 3.2E13 -0.17 0.44E3 !<ZHONG98>!
C5H5#+R2OH=>C4H6Z2+B2CO 4e14 0.0 4500 ! [PENGLOAN- RODA]

C5H5#+R2OH=C5H5OH# 1.0E13 0.0 0.0 !calculated!
C5H5#+R3OOH=C5H5O#+R2OH 3.0E12 0.0 0.0 !calculated!
!calculation by KINGAS!
!C5H5#+C5H5#=>C10H10# 2.0E12 0.0 0.0 !estimated!
!C10H10#=>C5H5#+C5H5# 3.2E15 0.0 57.5E3 !calculated!
!***disproportionnations!
C5H5#+R3OOH=>C5H6#+O2 2.5E9 1.0 3.5E3 !estimated!
!estimated as for allylic radicals (HEYBERGER02)/10!

!REACTIONS OF CYCLOPENTADIONYL RADICALS!

!***Decompositions by beta-scission!

C5H5O#=>2C2H2+R5CHO 2.0E13 0.0 30.0E3 !estimated!
C5H5O#=C5H4O#+R1H 2.0E13 0.0 30.0E3 !estimated!

!see DA COSTA01!

!***Combinations!

C5H5O#+R1H=C5H5OH# 1.0E14 0.0 0.0 !estimated!

!***no disproportionnations considered!

!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!

C5H4OH#+O2=C5H4O#+R3OOH 1.0E13 0.0 5.0E3 !estimated!
C5H4OH#+R1H=C5H5OH# 1.0E14 0.0 0.0 !estimated!
C5H4OH#+B10=C02+C2H2+R10C2H3V 3.2E13 -0.17 0.44E3 !estimated!
!C5H4OH#+R3OOH=>R2OH+CO2+R10C2H3V+C2H2 3.0E12 0.0 0.0 !estimated!
C5H4OH#+R3OOH=>R2OH+R2OH+C5H4O# 3.0E12 0.0 0.0 !mf

C5H4OH#+R3OOH=>C5H5OH#+O2 2.5E9 1.0 3.5E3 !estimated!

!Reactions derived from those of cyclopentadienyl radicals!

C5H4OH#+C6H5O#=C5H4O#+C6H5OH# 1.0E12 0.0 0.0 !estimated!

!Decomposition!

C5H5#=C2H2+aC3H3 2.79e79 -18.3 1.31e5 !Moskaleva/Lin 2000!

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

!REACTIONS OF ORTHOBENZOQUINONE!

OC6H4O=>C5H4O#+B2CO 1.0E12 0.0 40.0E3 !<ALZUETA00>!
 OC6H4O+R1H=>2B2CO+C2H2+R10C2H3V 5.2E13 0.0 3.2E3 !estimated!
 !estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
 OC6H4O+R1H=>H2+2B2CO+C2H2+R9C2H 1.6E6 2.5 9.8E3 !estimated!
 OC6H4O+R2OH=>H2O+2B2CO+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!
 !*****!

!C6H5OH#=C5H6#+B2CO 1.0E12 0.0 61.2E3 !<HORN98>!
 C6H5OH#=C5H6#+B2CO 2.67e14 -0.61 7.41e4 !<Xu,Lin2006>!

C6H5OH#+O2=R30OH+C6H5O# 1.0E13 0.0 38.9E3 !<ALZUETA00>!

C6H5OH#+B1O=OC6H4OH+R1H 1.6E13 0.0 3.4E3 !estimated!

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

C6H5OH#+R1H=C6H5O#+H2 1.2E14 0.0 12.4E3 !<ALZUETA00>!
 C6H5OH#+B1O=C6H5O#+R2OH 1.3E13 0.0 2.9E3 !<ALZUETA00>!
 C6H5OH#+R2OH=C6H5O#+H2O 1.4E8 1.4 -0.96E3 !<SHANDROSS96>!
 C6H5OH#+R30OH=C6H5O#+H2O2 1.0E12 0.0 10.0E3 !<ALZUETA00>!
 C6H5OH#+R4CH3=C6H5O#+CH4 1.8E11 0.0 7.7E3 !<MULCAHY65>!
 C6H5OH#+C6H5#=C6H5O#+C6H6# 4.9E12 0.0 4.4E3 !<ALZUETA00>!
 !C6H5OH#+C5H5#=C6H5O#+C5H6# 4.9E11 0.0 9.4E3 !estimated!
 !C6H5OH#+C3H5Y=C6H5O#+C3H6Y 4.9E11 0.0 9.4E3 !estimated!
 !C6H5OH#+iC4H5=C6H5O#+C4H6Z2 4.9E11 0.0 9.4E3 !estimated!
 C6H5OH#+C5H5#=C6H5O#+C5H6# 2.67e14 0.0 25.238e3 !mf <Lovell Int. J. Chem.
 Kinet.21(1989)547>
 C6H5OH#+C3H5Y=C6H5O#+C3H6Y 2.67e14 0.0 25.238e3 !mf <Lovell Int. J. Chem.
 Kinet.21(1989)547>
 C6H5OH#+iC4H5=C6H5O#+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!

C6H5OH#+R1H=C6H4OH#+H2 1.7E14 0.0 16.0E3 !<SHANDROSS96>!
 C6H5OH#+B1O=C6H4OH#+R2OH 2.0E13 0.0 14.7E3 !estimated!
 C6H5OH#+R2OH=C6H4OH#+H2O 1.4E13 0.0 4.6E3 !<SHANDROSS96>!
 C6H5OH#+R30OH=C6H4OH#+H2O2 4.0E11 0.0 28.9E3 !estimated!
 C6H5OH#+R4CH3=C6H4OH#+CH4 2.0E12 0.0 15.0E3 !estimated!

!as the H-abstractions from benzene!

C6H4OH#+O2=OC6H4OH+B1O 2.1E13 0.0 6.1E3 !estimated!
 !as for phenyl radicals (FRANCK94)!
 C6H4OH#+R1H=C6H5OH# 1.0E14 0.0 0.0 !estimated!
 C6H4OH#+R4CH3=HOC6H4CH3 5.0E12 0.0 0.0 !mf

!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!

C5H6#+O2=>C5H5#+R3OOH 1.4E12 0.0 31.6E3 !<INGHAM94>!
!C5H6#+R1H=C5H7# 5.2E13 0.0 3.2E3 !estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
C5H6#+B10=>C5H50#+R1H 8.9E12 -0.15 590.0 !<ZHONG98>!
!C5H6#+R1H=C5H5#+H2 2.8E13 0.0 2.0E3 !<ROY97>!
!C5H6#+R1H=C5H5#+H2 2.8E13 0.0 2.26E3 !<Horn>!
!C5H6#+R1H=C5H5#+H2 3.03e08 1.71 2811 !<Robinson2011>!
C5H6#+R1H=C5H5#+H2 6.67E+07 1.874 4259.0 !<CBSQB3>!
C5H6#+R1H=C3H5Y+C2H2 7.74E+36 -6.810 32918.7 !<ZHONG98>!
!C5H6#+R4CH3=C5H5#+CH4 3.51E+03 2.866 5655.0 !CBS-QB3!
C5H6#+R4CH3=C5H5#+CH4 3.11E+11 0.00 5500.0 !Pecullan ref49!
C5H6#+C3H3=C5H5#+aC3H4 0.80E+12 0.000 15100.0 !astoluene!
C5H6#+C3H3=C5H5#+pC3H4 0.80E+12 0.000 15100.0 !astoluene!
C5H6#+iC4H3=C5H5#+C4H4 1.60E+12 0.000 15100.0 !astoluene!
C5H6#+C5H7#Y=C5H5#+C5H8# 1.60E+12 0.000 15100.0 !astoluene!

!C5H6#+R1H=C3H5Y+C2H2 6.6e14 0.0 12.31E3 !<Horn>!

C5H6#+B10=C5H5#+R2OH 4.8E4 2.7 1.1E3 !<ZHONG98>!
C5H6#+R2OH=C5H5#+H2O 3.1E6 2.0 0.0 !<ZHONG98>!
C5H6#+R3OOH=C5H5#+H2O2 1.1E4 2.6 12.9E3 !<ZHONG98>!
!C5H6#+R4CH3=C5H5#+CH4 1.8E-1 4.0 0.0 !<ZHONG98>!
C5H6#+C3H5Y=C5H5#+C3H6Y 1.6E12 0.0 15.1E3 !astoluene!
C5H6#+nC4H5=C5H5#+C4H6Z2 1.6E12 0.0 11.1E3 !astoluene!
C5H6#+iC4H5=C5H5#+C4H6Z2 1.6E12 0.0 15.1E3 !astoluene!
!C5H6#+C3H5Y=C5H5#+C3H6Y 6.0E12 0.0 0.0 !estimated!
!C5H6#+nC4H5=C5H5#+C4H6Z2 6.0E12 0.0 0.0 !estimated!
!C5H6#+iC4H5=C5H5#+C4H6Z2 6.0E12 0.0 0.0 !<EMDEE92>!

!C5H7#=>C2H2+C3H5Y 2.0E13 0.0 35.5E3 !estimated!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by HEYBERGER02!
!C5H7#+O2=C5H6#+R3OOH 7.9E11 0.0 5.0E3 !estimated!
!oxidation of an alkylic radical!

!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!

C5H40#=>2C2H2+B2CO 5.7E32 -6.76 68.5E3 !<ALZUETA00>!
!C5H40#=B2CO+C4H4 1.00e12 0.0 53000 !roda PENGLOAN!
C5H40#+R1H=B2CO+nC4H5 2.6E13 0.0 3.2E3 !estimated!

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

C5H40#+B10=C4H4+CO2 1.0E13 0.0 2.0E3 !<ALZUETA00>!
C5H40#+R1H=C5H30#+H2 8.13E7 2.031 15.88E3 !MF idem C6H6#+R1H=C6H5#+H2
C5H40#+B10=C5H30#+R2OH 1.4E13 0.0 14.7E3 !<ALZUETA00>!
C5H40#+R2OH=C5H30#+H2O 1.1E8 1.42 1.4E3 !<ALZUETA00>!

C5H30#=>C2H2+B2CO+R9C2H 2.0E13 0.0 51.0E3 !estimated!

!estimated as the decomposition of lC6H5!

C5H30#+O2=>CO2+C2H2+R12CHCOZ 9.7E58 -13.47 38.2E3 !<ALZUETA00>!

C5H50H#+R1H=C5H50#+H2 4.0E13 0.0 6.1E3 !<ALZUETA00>!

C5H5OH#+B1O=C5H5O#+R2OH 1.0E13 0.0 4.6E3 !<ALZUETA00>!
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#+B1O=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+B1O=>R13CH2CHO+R12CHCOZ 6.0E4 2.56 -1.1E3 !estimated!
C4H4O+B1O=>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+B1O=>C2H2+R12CHCOZ+R2OH 1.2E11 0.7 8.7E3 !estimated!
C4H4O+B1O=>C3H3+B2CO+R2OH 6.0E10 0.7 8.7E3 !estimated!

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

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

!*****!
!* *!
!* 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+R3OOH 1.8E12 0.0 39.7E3 !<BAULCH94>!
!toluene+O2=benzyl+R3OOH 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+R2OH=HOC6H4CH3+R1H 2.3E12 0.0 -0.36E3 !<BAULCH92>!
toluene+R2OH=HOC6H4CH3+R1H 1.3E13 0.0 10.6E3 !<BAULCH94>as benzene!

toluene+R2OH=C6H5OH#+R4CH3 7.83E2 2.884 3.2193E3 !Seta V Nakajima V Miyoshi JPCA 2006
Zhenyu
!toluene+R2OH=C6H5OH#+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+R2OH 6.3E11 0.0 0.0 !<HOFFMANN90>!

toluene+R2OH=benzyl+H2O 5.2E09 1.0 0.87E3 !<BAULCH94>!

toluene+R3OOH=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+R7CH3O=benzyl+CH3OH 2.12E+10 0.0 3000.0 !PITZ2001
toluene+R8CH3OO=benzyl+CH3OOH 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+C6H5OOH

1.02E+04 2.5 12339.3 !PITZ2001

toluene+C6H5#=benzyl+C6H6# 7.9E13 0.0 12.0E3 !<HECKMANN96>!

toluene+C6H5O#=benzyl+C6H5OH# 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+C6H5CH2OO=benzyl+C6H5CH2OOH 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!

!**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+B1O=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+R3OOH=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+B1O 6.3E12 0.0 40.0E3 !<BREZYNSKY84>!

!**TERMINATION REACTIONS

benzyl+B1O=C6H5#+HCHO 3.5E13 0.0 0.0 !<EMDEE92>!

benzyl+B1O=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+R3OOH=C6H5CH2OOH 5.0E12 0.0 0.0 !<HIPPLER92>!
 benzyl+R3OOH=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+B1O=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 = $ekbT/h \times rpd \times \exp((Dnirotx3.5)/R)$, 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=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 = $ekbT/h \times rpd \times \exp((Dnirotx3.5)/R)$, 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 ROO. 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>!

!C6H6#+R1H=RMCPDY 5.22e28 -4.3 28.8e3 !Pecullan!
OC6H4CH3=B2CO+RMCPDY 7.4e11 0 43853 !Pecullan!

!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 *!

!*
*!

!*****!

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

! Amorage
!C6H5CHO+O2=C6H5CO+R3OOH 2.0E13 0.0 38.9E3 !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R3OOH 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+B1O=C6H5CO+R2OH 6.0E12 0.0 1.8E3 !<BAULCH94>!
C6H5CHO+R2OH=C6H5CO+H2O 7.8E12 0.0 0.0 !<BAULCH94>!
C6H5CHO+R3OOH=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>!
C6H5CO=C6H5#+B2CO 5.27E14 0.0 29.01e3 !<Nam,Lin,99>!

!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
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!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)>!
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!(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+R3OOH=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+R3OOH=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)>!
HOC6H4CH3+C5H5#=HOC6H4CH2+C5H6#	1.6E11	0.0	15.1E3	!<estimated(t)>!
HOC6H4CH3+C6H5#=HOC6H4CH2+C6H6#	7.9E13	0.0	12.0E3	!<estimated(t)>!
HOC6H4CH3+C6H5O#=HOC6H4CH2+C6H5OH#	1.6E11	0.0	15.1E3	!<estimated(t)>!
HOC6H4CH3+C6H4CH3=HOC6H4CH2+toluene	7.9E13	0.0	12.0E3	!<estimated(t)>!
HOC6H4CH3+OC6H4CH3=HOC6H4CH2+HOC6H4CH3		1.6E11	0.0	15.1E3
!<estimated(t)>!				

$\text{HOC6H4CH3} + \text{C6H5CH2OO} = \text{HOC6H4CH2} + \text{C6H5CH2OOH}$ 4.0E11 0.0 14.0E3
 !<estimated(t)>!
 $\text{HOC6H4CH3} + \text{C6H5CH2O} = \text{HOC6H4CH2} + \text{C6H5CH2OH}$ 1.6E11 0.0 11.1E3
 !<estimated(t)>!

$\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH2OO}$ 4.6E11 0.0 -377.0 !<estimated(u)>!
 $\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH2O} + \text{B1O}$ 6.3E12 0.0 40.0E3 !<estimated(u)>!
 $\text{HOC6H4CH2} + \text{R3OOH} = \text{HOC6H4CH2O} + \text{R2OH}$ 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)>!
 $\text{HOC6H4CH2} + \text{R4CH3} = \text{C6H5OH\#} + \text{C2H4Z}$ 5.0E12 0.0 0.0 !<estimated(g)>!

$\text{HOC6H4CH2OO} = \text{C6H4OHCHO} + \text{R2OH}$ 3.4E9 1.0 37.5E3 !<estimated(v)>!
 !(v) : Rate constant taken equal to that of the same reaction for benzyl peroxy radicals !

$\text{HOC6H4CH2O} = \text{R1H} + \text{C6H4OHCHO}$ 2.0E13 0.0 27.5E3 !<estimated(w)>!
 $\text{HOC6H4CH2O} = \text{C6H4OH\#} + \text{HCHO}$ 2.0E13 0.0 27.5E3 !<estimated(w)>!
 $\text{HOC6H4CH2O} + \text{O2} = \text{R3OOH} + \text{C6H4OHCHO}$ 6.0E10 0.0 1.6E3 !<estimated(w)>!
 !(w) : Rate constant taken equal to that of the same reaction for benzyl alcoxy radicals !

$\text{C6H4OHCHO} + \text{R1H} = \text{C6H4OHCO} + \text{H2}$ 4.0E13 0.0 3.2E3 !<estimated(x)>!
 $\text{C6H4OHCHO} + \text{B1O} = \text{C6H4OHCO} + \text{R2OH}$ 6.0E12 0.0 1.8E3 !<estimated(x)>!
 $\text{C6H4OHCHO} + \text{R2OH} = \text{C6H4OHCO} + \text{H2O}$ 7.8E12 0.0 0.0 !<estimated(x)>!
 $\text{C6H4OHCHO} + \text{R3OOH} = \text{C6H4OHCO} + \text{H2O2}$ 3.0E12 0.0 11.0E3 !<estimated(x)>!
 $\text{C6H4OHCHO} + \text{R4CH3} = \text{C6H4OHCO} + \text{CH4}$ 2.0E-6 5.6 1.5E3 !<estimated(x)>!
 !(x) : Rate constant taken equal to that of the same reaction for benzaldehyde !

$\text{C6H4OHCO} = \text{C6H4OH\#} + \text{B2CO}$ 2.0E13 0.0 30.5E3 !<estimated(y)>!
 !(y) : Rate constant taken equal to that of the same reaction for C6H5CO radicals !

!From Pecullan_1997

$\text{C6H5O\#} + \text{R4CH3} = \text{MCPD} + \text{B2CO}$ 2.05e75 -18.29 38.88e3 !Pecullan_1997!
 $\text{C6H5O\#} + \text{R4CH3} = \text{OC6H4CH3} + \text{R1H}$ 3.33e39 -7.78 31.67e3 !Pecullan_1997!
 $\text{C6H5O\#} + \text{R4CH3} = \text{HOC6H4CH3}$ 2.31e73 -17.37 38.78e3 !Pecullan_1997!
 $!\text{C6H5O\#} + \text{R4CH3} = \text{HOC6H4CH3}$ 2.31e72 -17.37 38.78e3 !Pecullan_1997!
 $\text{C6H5O\#} + \text{R4CH3} = \text{C6H4OH\#} + \text{R4CH3}$ 1.29e-31 13.2 15.58e3 !Pecullan_1997!

$!(\text{H})(\text{CH3})\text{C6H4O} = \text{C6H5O\#} + \text{R4CH3}$ 1.1e58 -12.27 35.19e3 !Pecullan_1997!
 $!\text{C6H5O\#} + \text{R4CH3} = (\text{H})(\text{CH3})\text{C6H4O}$ 2.28e86 -21.56 36.09e3 !Pecullan_1997!
 $!\text{C6H5O\#} + \text{R4CH3} = (\text{H})(\text{CH3})\text{C6H4O}$ 2.28e85 -21.56 36.09e3 !Pecullan_1997!
 $!(\text{H})(\text{CH3})\text{C6H4O} = \text{MCPD} + \text{B2CO}$ 1.18e47 -10.32 51.91e3 !Pecullan_1997!
 $!(\text{H})(\text{CH3})\text{C6H4O} = \text{HOC6H4CH3}$ 2.73e60 -13.73 64.3e3 !Pecullan_1997!

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

$\text{C6H5CH2OH} + \text{O2} = \text{R3OOH} + \text{C6H5CHOH}$ 1.4E12 0.0 34.0E3 !RODA <estimated(aaa)>!

!C6H5CH2OH+O2=C6H5CH2O+R3OOH 2.0E14 0.0 41.4E3 !<EMDEE92>!

C6H5CH2OH+R1H=C6H6#+R6CH2OH 5.8E13 0.0 8.1E3 !<estimated(t)>!

C6H5CH2OH+R1H=C6H5CHOH+H2 8.0E13 0.0 6.4E3 !<estimated(t')>!

C6H5CH2OH+B1O=C6H5CHOH+R2OH 4.2E11 0.0 -2.0E3 !<estimated(t')>!

C6H5CH2OH+R2OH=C6H5CHOH+H2O 3.5E9 1.0 -1.13E3 !<estimated(t')>!

C6H5CH2OH+R3OOH=C6H5CHOH+H2O2 2.7E11 0.0 12.0E3 !<estimated(t')>!

C6H5CH2OH+R4CH3=C6H5CHOH+CH4 1.1E12 0.0 9.1E3 !<estimated(t')>!

C6H5CH2OH+C3H5Y=C6H5CHOH+C3H6Y 1.1E12 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+iC4H5=C6H5CHOH+C4H6Z2 1.1E12 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+nC4H5=C6H5CHOH+C4H6Z2 1.112 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+C6H5#=C6H5CHOH+C6H6# 5.2E13 0.0 10.0E3 !<estimated(t')>!

C6H5CH2OH+C6H4CH3=C6H5CHOH+toluene 5.2E13 0.0 10.0E3 !<estimated(t')>!

C6H5CH2OH+C6H5O#=C6H5CHOH+C6H5OH# 1.1E11 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+benzyl=C6H5CHOH+toluene 1.1E11 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+OC6H4CH3=C6H5CHOH+HOC6H4CH3 1.1E11 0.0 13.1E3 !<estimated(t')>!

C6H5CH2OH+HOC6H4CH2=C6H5CHOH+HOC6H4CH3 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 0.0 36.373E3 !MF DHr=36.79 correlation baptiste

E=0.6*DHr+14.3

!R15C2H5O=CH3CHO+R1H 2.0E14 0.0 23.3E3 !(243,-243)<HEICKLEN88NIST>!

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

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

!** Amorçages bimoléculaires
 etC6H5+O2=C8H9#+R3OOH 1.4E12 0.0 34.0E3 !<estimated(aaa)>!
 etC6H5+O2=C8H9#-1+R3OOH 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+B1O=C8H9#+R2OH 4.2E11 0.0 -2.0
 !<estimated(t'')>!
 etC6H5+R2OH=C8H9#+H2O 3.5E9 1.0 -1.13E3 !<estimated(t'')>!
 etC6H5+R3OOH=C8H9#+H2O2 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 correlation Dean-Bozzelli 2000	7.2E8	1.5	6.79E3	!MF
etC6H5+B1O=C8H9#-1+R2OH correlation Dean-Bozzelli 2000	5.1E8	1.5	5.05E3	!MF
etC6H5+R2OH=C8H9#-1+H2O correlation Dean-Bozzelli 2000	3.6E6	2.0	4.82E2	!MF
etC6H5+R3OOH=C8H9#-1+H2O2 correlation Dean-Bozzelli 2000	4.2E4	2.69	1.85E4	!MF correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4 correlation Dean-Bozzelli 2000	2.43E6	1.87	1.03E4	!MF correlation Dean-Bozzelli 2000

!mfetC6H5+C6H5#=#C6H6#+C8H9#
<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+B1O=C6H5O#+R11C2H5 1.7E13 0.0 3.6E3 !MF as toluene !<TAPPE89>!

etC6H5+R2OH=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=R3OOH+styrene 6.90E11 0.0 15.2E3 !<est (exgas-sylvain)>!

!C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO 3.27E12 0.0 0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

```

!C8H9#+R3OOH=R2OH+R1H+C6H5COCH3          7.80E10    0.0    0.0
      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R3OOH=>R2OH+C6H5#+CH3CHO          2.54E11    0.0    0.0
      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R3OOH=C8H9#OOH                      3.60E12    0.0    0.0
      !MF KINGAS
C8H9#OOH=H2O+C6H5COCH3                    1.28E07                                2.25
      44950      !MF
C8H9#OOH=R2OH+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=R1H+C6H5COCH3                      9.77E12    0.0    17256
      !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=R3OOH+styrene          2.60E11    0.0    2.5E3
C8H9#-1+R3OOH=R2OH+HCHO+benzyl      5.00E12    0.0    0.0    !<kingas>!

!*****!
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!
!*****!

styrene+O2=R3OOH+C6H5C2H2          2.0E13    0.0    57.9E3    !<asbutadiene/2>!
!C4H6Z2+O2=iC4H5+R3OOH          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+R2OH=benzyl+HCHO          1.4E12    0.0    -0.9E3    !<as butadiene/2>!
styrene+R2OH=C6H5CHO+R4CH3        1.4E12    0.0    -0.9E3    !MF idem réaction précédente as
C3H6Y <TSAng91>

!C4H6Z2+B10=C3H5Y+R1H+B2CO        6.0E08    1.45    0.9E3    !<LEUNG95,BREZINSKY84>!
!C4H6Z2+R2OH=C3H5Y+HCHO          2.8E12    0.0    -0.9E3    !<LINSTEDT96>!
!C4H6Z2+R2OH=CH3CHO+R10C2H3V      5.6E12    0.0    -0.9E3    !<fromLINSTEDT96>!

styrene+R1H=C6H5C2H2+H2          3.3E5     2.53    9.2E3    !MF<as butadiene/2>!
styrene+R2OH=C6H5C2H2+H2O        1.5E6     2.0     0.4E3    !<as butadiene/2>!
styrene+R4CH3=C6H5C2H2+CH4        3.5E13    0.0     15.5E3    !<as butadiene/2>

styrene+B10=C6H5CH2CHO          1.5E08    1.45    0.9E3    !as butadiene / 2 /2!
styrene+B10=C6H5COCH3          1.5E08    1.45    0.9E3    ! as butadiene / 2 /2!
styrene+R3OOH=>C6H5CH2CHO+R2OH      1.0E12    0.0     14200
styrene+R3OOH=>C6H5COCH3+R2OH      1.0E12    0.0     14200.

!C4H6Z2+R1H=iC4H5+H2            6.6E5     2.53    9.2E3    !<WANG97>!
!C4H6Z2+R2OH=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#+R3OOH 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+R3OOH=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+R2OH=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+R3OOH 1.6E12 0.00 15200 !as allylique

C14H13#+R3OOH=>R2OH+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+R2OH=C6H5OH#+C6H5C2H2 7.83E2 2.884 3.2193E3 !Seta V Nakajima V Miyoshi JPCA
2006

! ajout MF

stilbene+R2OH=C6H5CHO+benzyl 1.0E13 0.0 5.94E3 !<Baulch05> as C2H4

!*****!

!*REACTIONS OF C6H5OCH2C6H5 *!

!*****!

!Ajout Ipso MF

C6H5OCH2C6H5+R1H=C6H5CH2O+C6H6# 8.51E12 0.0 5813 !

1990MAN/LOU4127-4134

C6H5CH2O+toluene=C6H5OCH2C6H5+R4CH3 7.8E2 2.884 3220

! ajout MF

C6H5O#+benzyl=C6H5OCH2C6H5 1.0E11 0.0 0.00

! ajout MF

C6H5OCH2C6H5+R2OH=>C6H5#+C6H5CHO+H2O 3.5E09 1.0 0.87E3 ! 2/3 as toluene

C6H5OCH2C6H5+R1H=>C6H5#+C6H5CHO+H2 1.95E6 2.372 5.81E3 ! 2/3 as toluene

C6H5OCH2C6H5+B1O=>C6H5#+C6H5CHO+R2OH 4.2E11 0.0 0.0 ! 2/3 as toluene

!*****!

!*REACTIONS OF TolOCH2C6H5 *!

!*****!

!Ajout Ipso MF

TolOCH2C6H5+R1H=toluene+C6H5CH2O 8.51E12 0.0

5813 ! 1990MAN/LOU4127-4134

! ajout MF

OC6H4CH3+benzyl=TolOCH2C6H5 1.0E11 0.0 0.00

!

C6H4CH3+C6H5CH2O=TolOCH2C6H5 1.0E11 0.0 0.00 !

! ajout MF

TolOCH2C6H5+R2OH=>C6H4CH3+C6H5CHO+H2O 8.75E09 1.0 0.87E3 ! 5/3 as toluene
 TolOCH2C6H5+R1H=>C6H4CH3+C6H5CHO+H2 4.875E6 2.372 5.81E3 ! 5/3 as
 toluene
 TolOCH2C6H5+B10=>C6H4CH3+C6H5CHO+R2OH 10.5E11 0.0 0.0 ! 5/3 as toluene

!*****!

!*REACTIONS OF PhenolCH2bz *!

!*****!

!Ajout Ipso MF negligible

!C6H5OH#+benzyl=PhenolCH2bz+R1H 1.0E12 0.0 0.00 !

!HOC6H4CH2+C6H6#=PhenolCH2bz+R1H 1.0E12 0.0 0.00 !

! ajout MF

C6H4OH#+benzyl=PhenolCH2bz 1.0E13 0.0 0.00 !

HOC6H4CH2+C6H5#=PhenolCH2bz 1.0E13 0.0 0.00 !

! ajout MF

PhenolCH2bz+R1H=>C6H5OH#+C4H2+pC3H4+H2 2.92E6 2.372 5.81E3 !AS

TOLUENE

PhenolCH2bz+B10=>C6H5OH#+C4H2+pC3H4+R2OH 6.3E11 0.0 0.0 !AS

TOLUENE

PhenolCH2bz+R2OH=>C6H5OH#+C4H2+pC3H4+H2O 5.2E09 1.0 0.87E3 !AS

TOLUENE

!*****!

!*REACTIONS OF PhenolC2H4bz *!

!*****!

!Ajout Ipso MF

! negligible C6H5OH#+C8H9#-1=PhenolC2H4bz+R1H

bibenzyl+R2OH=PhenolC2H4bz+R1H 1.7E13 0.0 10600 ! as benzene

+ OH x10/6

! ajout MF

C6H4OH#+C8H9#-1=PhenolC2H4bz 1.0E11 0.0 0.00 !

HOC6H4CH2+benzyl=PhenolC2H4bz 1.0E11 0.0 0.00 !

! ajout MF

PhenolC2H4bz+R2OH=>styrene+C6H5OH#+H2O 8.75E09 1.0 0.87E3 ! 5/3 as toluene

PhenolC2H4bz+R1H=>styrene+C6H5OH#+H2 4.875E6 2.372 5.81E3 ! 5/3 as

toluene

PhenolC2H4bz+B10=>styrene+C6H5OH#+R2OH 10.5E11 0.0 0.0 ! 5/3 as toluene

!*****!

!*REACTIONS OF Benzaldtol *!

!*****!

!Ajout Ipso MF negligible

!C6H5CO+HOC6H4CH3=Benzaldtol+R1H

! ajout MF

C6H5CO+OC6H4CH3=Benzaldtol 3.0E12 0.0 0.00 !

! ajout MF

Benzaldtol+R2OH=>C6H5CHO+C6H5CO+H2O 5.2E09 1.0 0.87E3 !AS TOLUENE
 Benzaldtol+R1H=>C6H5CHO+C6H5CO+H2 2.92E6 2.372 5.81E3 !AS TOLUENE
 Benzaldtol+B10=>C6H5CHO+C6H5CO+R2OH 6.3E11 0.0 0.0 !AS TOLUENE

!*****!
 !*REACTIONS OF HOC6H4CHO. *!
 !*****!

! ajout MF
 HOC6H4CH2+O2=HOC6H4CHO+R2OH 6.3E12 0.00 40000
 ! AS BENZYL+O2
 HOC6H4CH2+R3OOH=>HOC6H4CHO+R2OH+R1H 8.21e4 2.20 -5130
 ! AS BENZYL+HO2

! ajout MF
 HOC6H4CHO+R2OH=>B2CO+C6H5O#+H2O 3.5E09 1.0 0.87E3 !AS PHENOL
 DUP
 HOC6H4CHO+R1H=>B2CO+C6H5O#+H2 1.95E6 2.372 5.81E3 !AS PHENOL
 DUP
 HOC6H4CHO+B10=>B2CO+C6H5O#+R2OH 4.2E11 0.0 0.0 !AS PHENOL
 DUP

HOC6H4CHO+R2OH=>B2CO+C6H5O#+H2O 7.8E12 0.0 0.0 !AS C6H5CHO
 DUP
 HOC6H4CHO+R1H=>B2CO+C6H5O#+H2 4.0E13 0.0 3.2E3 !AS C6H5CHO
 DUP
 HOC6H4CHO+B10=>B2CO+C6H5O#+R2OH 6.0E12 0.0 1.8E3 !AS C6H5CHO
 DUP

!*****!
 !*REACTIONS OF C6H5C4H7 *!
 !*****!

benzyl+C3H5=C6H5C4H7 5.0E12 0.00 0.00

! ajout MF
 C6H5C4H7+R2OH=>benzyl+pC3H4+H2O 5.2E09 1.0 0.87E3 !AS 2/3TOLUENE
 wrong products but Y rad
 DUP
 C6H5C4H7+R1H=>benzyl+pC3H4+H2 2.92E6 2.372 5.81E3 !AS 2/3TOLUENE
 wrong products but Y rad
 DUP
 C6H5C4H7+B10=>benzyl+pC3H4+R2OH 6.3E11 0.0 0.0 !AS 2/3TOLUENE wrong
 products but Y rad
 DUP

C6H5C4H7+R2OH=>benzyl+pC3H4+H2O 3E6 2.0 -1520 !AS 2Hs allyl wrong products
 but Y rad
 DUP
 C6H5C4H7+R1H=>benzyl+pC3H4+H2 5.4E4 2.5 -1900 !AS 2Hs allyl wrong products
 but Y rad
 DUP
 C6H5C4H7+B10=>benzyl+pC3H4+R2OH 8.8E10 0.7 3250 !AS 2Hs allyl wrong products
 but Y rad

DUP

!*****!

!* REACTIONS OF Benzofuran *!

!*****!

C6H5O#+C2H2=>benzofuran+R1H 1.2E10 0.0 0.46E3 !TEST MF/10 analog oh+c2h2 base
nist!

!mfbenzofuran+R1H=C6H5O#+C2H2 5.67E8 1.43 5.65E3

C8H8O#+R1H=C6H5O#+C2H4Z 5.67E8 1.43 5.65E3 !as toluene+H
R1H+C8H7O#=C8H8O# 1.0E14 0.0 0.0E3

C8H8O#+R1H=C8H7O#+H2 9.6E6 2.0 5000 !AS
ETHYLBZ

C8H8O#+B10=C8H7O#+R2OH 1.6E13 0.0 5200 !AS
ETHYLBZ

C8H8O#+R2OH=C8H7O#+H2O 2.6E6 2.0 -770 !AS ETHYLBZ
C8H8O#+R4CH3=C8H7O#+CH4 2.0E11 0.0 9600 !AS ETHYLBZ

C8H8O#+R1H=C8H7O#-1+H2 8.0E13 0.0 6.4E3 !AS
ETHYLBZ

C8H8O#+B10=C8H7O#-1+R2OH 4.2E11 0.0 -2.0 !AS
ETHYLBZ

C8H8O#+R2OH=C8H7O#-1+H2O 3.5E9 1.0 -1.13E3 !AS ETHYLBZ
C8H8O#+R4CH3=C8H7O#-1+CH4 1.1E12 0.0 9.1E3 !AS ETHYLBZ

C8H7O#=benzofuran+R1H 3.30E10 0.885 35.77E3 ! as indanyl=indene+H
R1H+C8H7O#-1=C8H8O# 1.0E14 0.0 0.0E3

C8H7O#-1=benzofuran+R1H 1.21E11 0.985 42.2E3 ! as indanyl=indene+H

C8H7O#+O2=benzofuran+R3OOH 1.58E12 0.0 5.0E3 ! as indanyl
C8H7O#-1+O2=benzofuran+R3OOH 1.58E12 0.0 15.2E3 ! as indanyl

benzofuran+R2OH=>C6H4CH3+CO2 1.37E12 0.0 -1.04E3 !Touchard (add on double bond)!

benzofuran+R2OH=>C6H5CO+HCHO 1.37E12 0.0 -1.04E3

benzofuran+B10=>C6H5CO+B2CO+R1H 6.00E4 2.56 -1.13E3

!*****!

!* Reactions of naphthalene *!

!*****!

!2C5H5#=naphthalene+H2 4.3E36 -6.3 45.37E3 ! A.M. Dean, J. Phys. Chem. 94 (1990) 1432-1439.
Ea modif

!2C5H5#=naphthalene+H2 21.5E36 -6.3 45.37E3 ! A.M. Dean, J. Phys. Chem. 94 (1990) 1432-
1439. Ea modif; a*5

2C5H5#=naphthalene+2R1H 2E13 0.0 4e3 !Horn98!

!2C5H5#=naphthalene+2R1H 4.3E13 0.0 9.7e3 !Slavinskaya 2009!

C6H5#+iC4H3=naphthalene 3.18E23 -3.2 4.23E3 ! H.Y. Zhang, J.T. McKinnon, CST 107 (1995)
261-300. Ea modif

C6H5#+C4H4=naphthalene+R1H 3.3E33 -5.7 25.5E3 !J. Appel, H. Bockhorn, M. Frenklach,
Combust. Flame 121 (2000) 122-136.Ea modif
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 6.56E3 ! J. Appel, H. Bockhorn, M. Frenklach,
Combust. Flame 121 (2000) 122-136.Ea modif
C6H6#+C6H4#=naphthalene+C2H2 5.809e3 2.526 -5.919e3 !Comandini,Brezinsky J.Phys.Chem
2011,115,5547-5559

naphthalene+O2=R3OOH+naphthyl 8.0E13 0.0 63.4E3 !like benzene <ALZUETA00>A*8/6!
naphthalene+B1O=>indenyl+B2CO+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+B1O=naphthyl+R2OH 2.7E13 0.0 14.7E3 !like benzene
<LINDSTEDT94>A*8/6!
naphthalene+R2OH=naphthyl+H2O 2.1E8 1.42 1.45E3 !like benzene <BAULCH92>A*8/6!
naphthalene+R3OOH=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+B1O 2.6E13 0.0 6.1E3 !as n-buthylbenzene
naphthyl+B1O=>indenyl+B2CO 1.0E14 0.0 0.0 !as n-buthylbenzene
naphthyl+R3OOH=>indenyl+B2CO+R2OH 5.0E12 0.0 0.0 !as n-buthylbenzene
naphthyl+R2OH=>indenyl+B2CO+R1H 1.0E13 0.0 0.0 !as n-buthylbenzene

indenyl+C5H5#=>phenanthrene+2R1H 4.3E13 0.0 9.71E3 !in Slavinskaya09 A/10 Ea mod A*10

!*****!

!formation du naphthalene en passant par 9.10-dihydrofulvalene_Mebel 2009!

!*****!

!2C5H5#=S0 5E12 0 0

!S0+R1H=C5H6#+C5H5# 2e13 0 1.3e3 !2*ipso addition de R1H sur MCPD
!S0+R4CH3=MCPD+C5H5# 38.56E10 0 8000 !4*addition de R4CH3 sur la double liaison!

!S0+R1H=>naphthalene+H2+R1H 13.34e7 1.874 4259 !2* methathese de C5H6#+R1H
!S0+R4CH3=>naphthalene+CH4+R1H 6.22e11 0 5500 !2* methathese de C5H6#+R4CH3
!S0+C5H5#=>naphthalene+C5H6#+R1H 1.07e11 0 15.1e3 !(2/3)* methathese de
toluene+C5H5#

!*****!

!* Reactions of indene and derived radicals *!

! Indene C6H4#/CH2/CH//CH/ *!

! Indenyl C6H4#/CH/CH//CH/ *!

! ph#C3H2 C6H5#/CH(./C//CH *!

!*****!

indene+R2OH=>C2H4Z+C6H5CO 1.37E12 0.0 -1.04E3 !Slavinskaya

indene+R2OH=>R10C2H3V+B2CO+C6H6# 1.37E12 0.0 -1.04E3 !Est.

indene+R2OH=>o-methylbenzyl+B2CO 1.37E12 0.0 -1.04E3

indene+O2=R3OOH+indenyl 1.4E12 0.0 31.03E3 ! as n-buthylbenzene mais E = DH de
reaction
indene+B10=indenyl+R2OH 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+R2OH=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+R3OOH=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 74.450E3 !Slavinskaya09 5.0E13 0.0 37.5E3 Ea modif
indenyl+R1H=indene 1.0E14 0.0 0.0 !as n-buthylbenzene
C6H5#+C3H3=indene 6.46E12 0.0 0.0 !Slavinskaya09
indenyl+R3OOH=>C6H6#+B2CO+R9C2H+R2OH 3.0E12 0.0 0.0 ! Est.!similar to C5H5#+HO2
indenyl+R3OOH=>C6H5#C2H+R5CHO+R2OH 3.0E12 0.0 0.0 ! Est.!similar to C5H5#+HO2

indenyl+B10=>C6H6#+B2CO+R9C2H 5.8E13 -0.02 0.02E3 !Est. C5H5#+B10=C5H4O#+R1H
indenyl+B10=>C6H5#C2H+R5CHO 5.8E13 -0.02 0.02E3 !Est. C5H5#+B10=C5H4O#+R1H

indenyl+R2OH=>styrene+B2CO 4.0E14 0.0 4.5E3 !Est. C5H5#+OH=C4H6Z2+CO

!C9H7O#=C9H6O#+R1H 2.0E13 0.0 27.5E3 ! Est.like ph#CH2O
!C9H7O#=>C6H6#+B2CO+R9C2H 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+CO
!C9H7O#=C6H5#C2H+R5CHO 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+CO

!*****
!* REACTIONS OF CUMENE !!
!*****

!**Unimolecular initiation

C8H9#+R4CH3=cumene 1E12 0.0 0.0 !A optimisé par MF
C6H5#+iC3H7=cumene 1E12 0.0 0.0 !A optimisé par MF

!**Bimolecular initiation

cumene+O2=>CH3styre+R1H+R3OOH 1.4E12 0.0 33.62E3 !estimated (Thergas)!
cumene+O2=C9H11#-1+R3OOH 2.4E13 0.0 52.3E3 !estimated (analog etC6H5)!

!**METATHESES

B10+cumene=R2OH+C9H11#-1 10.2E+13 0.0 7.85E3
cumene+R1H=H2+C9H11#-1 57.0E+06 2.0 7.70E3
cumene+R2OH=H2O+C9H11#-1 53.4E+05 2.0 0.45E3
cumene+R3OOH=H2O2+C9H11#-1 12.0E+11 0.0 17.0E3
cumene+R4CH3=CH4+C9H11#-1 6.0E-01 4.0 8.2E3

!mfcumene+B10=>R2OH+CH3styre+R1H 3.4E+10 0.7 1.33E3 ! Touchard!
!mfcumene+R1H=>H2+CH3styre+R1H 2.5E+04 2.5 -2.79E3

```

!mfcumene+R2OH=>H2O+CH3styre+R1H      1.3E+06  2.0  -2.62E3
!mfcumene+R3OOH=>H2O2+CH3styre+R1H     1.6E+04  2.6  10.9E3
!mfcumene+R4CH3=>CH4+CH3styre+R1H      5.0E+10  0.0  5.6E3

cumene+B10=>R2OH+CH3styre+R1H          2.1E+11  0.0  0  ! as toluene A/3
cumene+R1H=>H2+CH3styre+R1H            0.97E+06  2.372  5.81E3 ! as toluene A/3
cumene+R2OH=>H2O+CH3styre+R1H          1.73E+09  1.0  0.87E3 ! as toluene A/3
cumene+R3OOH=>H2O2+CH3styre+R1H        1.33E+11  0.0  14.0E3 ! as toluene A/3
cumene+R4CH3=>CH4+CH3styre+R1H         1.3  3.76  6.98E3 ! as toluene A/3

C9H11#-1=styrene+R4CH3      2.0E+13  0.0  31.0E3 ! Touchard!
C9H11#-1=C3H6Y+C6H5#        2.0E+13  0.0  38.5E3 !Beta-sciss EvansPolani corr(Ea=18.9+0.53drH)!
C9H11#-1=CH3styre+R1H      1.6E+13  0.0  34.3E3 ! Touchard!

C9H11#-1+O2=CH3styre+R3OOH          7.5E10  0.0          2500

C9H11#-1+R1H=cumene      1.0E+14  0.0  0.0  !<Allara80>touchard!

!*****!
!* REACTIONS OF CH3styre !!
!*****!

!**metatheses
CH3styre+R1H=C2H3C6H4CH2+H2  1.7E05  2.5  2.5E3  !Est similar to C5H8+R1H=C5H7Y+H2!
CH3styre+R2OH=C2H3C6H4CH2+H2O  3.0E06  2.0  -0.298E3 !Est.similar to C5H8+R2OH=C5H7Y+H2O!

C6H5C2H2+R4CH3=CH3styre      4E11  0.0  0.0  !
!CH3styre+R1H=styrene+R4CH3  5.8E13  0.0  8.1E3  !<BAULCH94> (Toluene)!
!CH3styre+R1H=toluene+R10C2H3V  5.8E13  0.0  8.1E3  !ipso-addition

!CH3styre+R1H=styrene+R4CH3  7.2E13  0.0  5.1E3  !S.Gail CaF141(2005)281-297
!CH3styre+R1H=toluene+R10C2H3V  2.4E13  0.0  5.1E3  !S.Gail CaF141(2005)281-297

!**Bimolecular initiation
CH3styre+O2=>aC3H4+C6H5#+R3OOH  1.2E13  0.0  49.0E3  !estimated (analogue etC6H5)!

!**METATHESES-Decompositions
B10+CH3styre=>R2OH+aC3H4+C6H5#  5.1E+13  0.0  7.85E3  ! Touchard
CH3styre+R1H=>H2+aC3H4+C6H5#  28.5E+06  2.0  7.70E3
CH3styre+R2OH=>H2O+aC3H4+C6H5#  26.7E+05  2.0  0.45E3
CH3styre+R3OOH=>H2O2+aC3H4+C6H5#  6.0E+11  0.0  17.0E3
CH3styre+R4CH3=>CH4+aC3H4+C6H5#  3.0E-01  4.0  8.2E3

!*****!
!* REACTIONS OF C6H5CH2CHO !!
!*****!
!AJOUTS REACTION RODA :
benzyl+R5CHO = C6H5CH2CHO          1.0E13  0.0  0.0

```

C6H5CH2CHO+R1H=>H2+B2CO+benzyl 4.0E13 0.0 4.2E3 !Butane mechanism
 C6H5CH2CHO+R2OH=>H2O+B2CO+benzyl 4.2E12 0.0 0.5E3 !Butane mechanism
 C6H5CH2CHO+R3OOH=>H2O2+B2CO+benzyl 1.0E12 0.0 10.0E3 !Butane mechanism
 C6H5CH2CHO+R4CH3=>CH4+B2CO+benzyl 2.0E-6 0.0 2.5E3 !Butane mechanism
 C6H5CH2CHO+R11C2H5=>C2H6+B2CO+benzyl 1.3E12 0.0 8.5E3 !Butane mechanism

!*****!

!* REACTIONS OF C6H5COCH3 !!

!*****!

C6H5COCH3+R1H=>H2+CH2COZ+C6H5# 2.8E7 2.0 7700 !exgas
 C6H5COCH3+R2OH=>H2O+CH2COZ+C6H5# 2.7E6 2.0 450 !exgas
 C6H5COCH3+R3OOH=>H2O2+CH2COZ+C6H5# 6.0E11 0.0 17000 !exgas
 C6H5COCH3+R4CH3=>CH4+CH2COZ+C6H5# 3.0E-1 4.0 8200 !exgas
 !C6H5COCH3+R11C2H5=>C2H6+CH2COZ+C6H5# 3E11 0.0 13500 !exgas

!***** AJOUT meca ANISOLE repris du butyl benzene Emir Pousse

!*****

!* REACTIONS OF Anisole !!

!*****

C6H5O#+R4CH3=anisole 5.0E12 0.0 0.0 !estimated (analogie etC6H5)!
 C6H5#OCH2+R1H=anisole 1.0E14 0.0 0.0 !estimated R+H Allara1980

!**Bimolecular initiation

anisole+O2=C6H5#OCH2+R3OOH 2.1E13 0.0 47.9E3 !estimated (analogie etC6H5)!

!IpsO addition

!anisole+R1H=C6H6#+R7CH3O 5.8E13 0.0 8.1E3 !<BAULCH94>! as toluene

anisole+R1H=C6H6#+R7CH3O 2.23e13 0.0 7930 !as phenol

anisole+R2OH=C6H5OH#+R7CH3O 7.8E02 2.88 3.22E3 ! as toluene +OH=phenol+ch3

Seta2006 NIST

!anisole+R4CH3=toluene+R7CH3O

!toluene+R7CH3O=anisole+R4CH3 7.8E02 2.88 3.22E3 ! as toluene +OH=phenol+ch3 Seta2006

NIST

!toluene+R7CH3O=anisole+R4CH3

3.9E02 2.88 3.22E3 ! as toluene +OH=phenol+ch3 Seta2006

NIST

anisole+R4CH3=toluene+R7CH3O 9.64e10 0.0 8e03 ! as addition of CH3 on C=C PAG

!anisole+R1H=C6H5OH#+R4CH3 0.1e14 0 6e3 !Ranzi!

!**METATHESES

B10+anisole=R2OH+C6H5#OCH2 3.0E+13 0.0 3.28E3 ! as 3 H tertiaire Exgas

!anisole+R1H=H2+C6H5#OCH2 12.6E+06 2.0 2.40E3 ! as 3 H tertiaire Exgas

!anisole+R1H=H2+C6H5#OCH2 7.2e08 1.5 4735 ! Evans Polanyi

anisole+R1H=H2+C6H5#OCH2 3.6e08 1.5 5735 ! Evans Polanyi

!anisole+R2OH=H2O+C6H5#OCH2 3.3E+06 2.0 -1.87E3 ! as 3 H tertiaire Exgas

anisole+R2OH=H2O+C6H5#OCH2 3.6e+06 2.0 -855 ! Evans Polanyi

!anisole+R3OOH=H2O2+C6H5#OCH2 3.0E+12 0.0 14.0E3 ! as 3 H tertiaire Exgas

anisole+R3OOH=H2O2+C6H5#OCH2	4.2e3	2.69	16592.2	!Evans Polanyi
!anisole+R4CH3=CH4+C6H5#OCH2	3.0E+11	0.0	7.9E3	!as 3 H tertiaire Exgas
!anisole+R4CH3=CH4+C6H5#OCH2	24.3e5	1.87	8260	!Evans Polanyi
anisole+R4CH3=CH4+C6H5#OCH2	5.01e11	0	1.05e4	!Mulcahy
anisole+R11C2H5=C2H6+C6H5#OCH2	3.0E+11	0.0	9.2E3	!as 3 H tertiaire Exgas
anisole+C5H5#=C5H6#+C6H5#OCH2	5.4E+00	3.3	17.2E3	!as 3 H tertiaire par Y. Exgas
!anisole+C6H5#=C6H6#+C6H5#OCH2	8.4E+11	0.0	3.0E3	!as 3* C6H5+Ht in C4H10 Park99
NIST				
anisole+C6H5#=C6H6#+C6H5#OCH2	3E+11	0.0	3851	!as 3* H secondary in C3H8+phenyl
Park2004 NIST				
C6H5OH#+C6H5#OCH2=anisole+C6H5O#	1.8E+11	0.0	7.7E3	!as C6H5OH+CH3 Mulcahy65
NISTervoir				
! Radical decomposition				
C6H5#OCH2=HCHO+C6H5#	2.61E+14	0.054	39.28E3	!Silva et Bozzelli 2009 (ancien
correlation EV BS 2007)				
C6H5#OCH2=C6H5CH2O	8.78e10		0.442	19.03e3 !Silva et Bozzelli
2009				
C6H5CH2O=C6H5CHO+R1H	5.26e28	-5.081	22.25e3	!Silva et Bozzelli 2009
!C6H5CH2O=C6H5CHO+R1H	5.26e28	-5.081	25.25e3	!Silva et Bozzelli 2009
+3kcal				
C6H5CH2O=C6H6# + R5CHO	2.37e32	-6.095	28.81e3	!Silva et Bozzelli 2009
C6H5CH2O=C6H5# + HCHO	7.21e33	-6.21	36.85e3	!Silva et Bozzelli 2009
C6H5CH2O+R1H=C6H5CH2OH	1e14	0.0	0.0	!estimated
C6H5CH2O+R4CH3=C6H5CHO + CH4	1e12	0.0	0.0	!estimated
C6H5CH2O+R1H=C6H5CHO + H2	1e13	0.0	0.0	!estimated
C6H5CH2O+C6H5#=C6H5CHO + C6H6#	1e12	0.0	0.0	!estimated
!C6H5#OCH2=C6H5CHO+R1H	3.16e+12	0.0	21.5e3	!Pecullan react n°4
!C6H5O#=B2CO+C5H5#	7.4e11	0.00	43853	!Pecullan (existe deja)
!*****				
!* REACTIONS OF Guaiacol !!				
!*****				
anisole+R2OH=guaiacol+R1H	0.65e13	0.0	10.6e3	!estimated from C6H6#+R2OH with
A/2!				
OC6H4OH+R4CH3=guaiacol	0.5e12	0	0	

!*****

!* Benzofuran from HOC6H4CH2 !!

!*****

HOC6H4CH2+R4CH3=HOC6H5#C2H5 5E12 0 0

HOC6H5#C2H5+R1H =HOC6H5#C2H4+H2 8e13 0 6.4e3 !estimated from etC6H5!
HOC6H5#C2H5+R2OH =HOC6H5#C2H4+H2O 3.5e9 1 -1.13e3 !estimated from etC6H5!
HOC6H5#C2H5+B10 =HOC6H5#C2H4+R2OH 4.2e11 0 -2 !estimated from etC6H5!
HOC6H5#C2H5+R4CH3 =HOC6H5#C2H4+CH4 1.1e12 0 9.1e3 !estimated from etC6H5!
HOC6H5#C2H5+C5H5# =HOC6H5#C2H4+C5H6# 1.1e11 0 13.1e3 !estimated from etC6H5!
HOC6H5#C2H5+C6H5# =HOC6H5#C2H4+C6H6# 5.27e13 0 12e3 !estimated from toluene!
HOC6H5#C2H5+C6H5O# =HOC6H5#C2H4+C6H5OH# 1.1e11 0 13.1e3 !estimated from
etC6H5!
HOC6H5#C2H5+benzyl=HOC6H5#C2H4+toluene 1.1e11 0 13.1e3 !estimated from etC6H5!

HOC6H5#C2H4=HOstyrene+R1H 3.1e13 0 50670 !estimated from styrene!

HOstyrene+R1H=benzofuran+H2+R1H 1.2e14 0 12.4e3 !estimated from phenol!
HOstyrene+R2OH=benzofuran+H2O+R1H 1.4e8 1.4 -0.96e3 !estimated from phenol!
HOstyrene+B10=>benzofuran+R2OH+R1H 1.3e13 0 2.9e3 !estimated from phenol!
HOstyrene+R4CH3=benzofuran+CH4+R1H 1.8e11 0 7.7e3 !estimated from phenol!
HOstyrene+C5H5#=>benzofuran+C5H6#+R1H 2.67e14 0 25.24e3 !estimated from phenol!
HOstyrene+C6H5# =benzofuran+C6H6#+R1H 4.9e12 0 4.4e3 !estimated from phenol!
HOstyrene+C6H5O#=>benzofuran+C6H5OH#+R1H 4.9e11 0 9.4e3 !estimated from cresol!
!HOstyrene+benzyl=benzofuran+toluene

!*****

!*****

!* Primary mechanism of the oxidation of indane *!

!*****

!*****

!*****

!* Reactions of indane *!

!*****

!**unimolecular initiation

!*rupture of C-C and C-H

indane=>CH3styre 1.26E16 0.0 84.9E3 ! Est.!W.Tsang,Int.J.Chem.Kin.10(1978)599-617

! by analogy with c-C5H10 TSA78!

R1H+indanyl-Y=indane 1.0E14 0.0 0.0 ! Est.R1H+C5H7#Y=C5H8#

R1H+indanyl-1=indane 1.0E14 0.0 0.0 ! Est.R1H+C5H7#=C5H8#

!**bimolecular initiation

indane+O2=indanyl-Y+R3OOH 2.8E12 0.0 35.96E3 ! Est.C5H8#+O2=C5H7#Y+HO2 A*2 delta H cal

indane+O2=indanyl-1+R3OOH 1.4E13 0.0 45.46E3 ! Est.C5H8#+O2=C5H7#+HO2 delta H cal

!**ipso-additions

indane+R1H=ph#C3H6-1 2.32E14 0.0 8.1E3 !nBB A*4
indane+R4CH3=CH3C6H4C3H6 2.4E12 0.0 15.9E3 !ph#C4H9+R4CH3=toluene+R20C4H9!A*2
indane+B1O=>C6H5O#+C3H5Y 1.7E13 -0.15 3.6E3 !toluene+O Tsang 1989

!**metatheses

!*metatheses with abstraction of H-atom

indane+R1H=indanyl-Y+H2 1.08E5 2.5 -1.9E3 !Est.!C5H8#+R1H=C5H7#Y+H2
indane+R1H=indanyl-1+H2 9.0E6 2.0 5.0E3 !Est.!C5H8#+R1H=C5H7#+H2

indane+B1O=indanyl-Y+R2OH 1.7E11 0.7 3.25E3 !Est.!C5H8#+O=C5H7#Y+OH
indane+B1O=indanyl-1+R2OH 2.6E13 0.0 5.2E3 !Est.!C5H8#+O=C5H7#+OH

indane+R2OH=indanyl-Y+H2O 6.0E6 2.0 -1.52E3 !Est.!C5H8#+OH=C5H7#Y+H2O
indane+R2OH=indanyl-1+H2O 2.6E6 2.0 -0.77E3 !Est.!C5H8#+OH=C5H7#+H2O

indane+R3OOH=indanyl-Y+H2O2 1.28E04 2.6 12.4E3 !Est.!ph#C4H9+R3OOH=ph#C4H8X+H2O2
indane+R3OOH=indanyl-1+H2O2 4.0E11 0.0 15.5E3 !Est.!ph#C4H9+R3OOH=ph#C4H8-3+H2O2

indane+R4CH3=indanyl-Y+CH4 2.0E11 0.0 7.3E3 !Est.!C5H8#+CH3=C5H7#Y+CH4
indane+R4CH3=indanyl-1+CH4 2.0E11 0.0 9.6E3 !Est.!C5H8#+CH3=C5H7#+CH4

indane+C6H5#=indanyl-Y+C6H6# 8E12 0.0 8.0E3 !Est.!toluene+C2H3#=benzyl+C2H4# A*2
indane+benzyl=indanyl-Y+toluene 8.8E12 0.0 13.1E3!Est.!ph#C4H9+benzyl=ph#C4H8X+toluene
A*2*4

!*****!

!* Reactions of indanyl-Y c(#1)&c(#2)&ch&ch&ch&ch&1,1/CH(./)CH2/CH2/2 *!

!*****!

!**bete-scission decomposition

indanyl-Y=C2H3C6H4CH2 1.36E12 0.440 41.33E3 !cal.
indanyl-Y=indene+R1H 1.21E11 0.985 42.2E3 !Cal.

!**combinations

indanyl-Y+R3OOH=>C9H9O#+R2OH 1.0E13 0.0 0.0 !Est.! Ph#C4H8X+R3OOH A*2
indanyl-Y+B1O=C9H9O# 1.16E14 -0.02 0.02E3!indenyl+B1O=C9H7O# A*2
indanyl-Y+R4CH3=methylindane 1.0E13 0.0 0.0 !Est.!C5H5#+R4CH3=MCPD A*2
indanyl-Y+benzyl=toluene+indene 1.0E13 0.0 0.0 !ph#C4H8X+benzyl=toluene+ph#C4H7-3 A*2
indanyl-Y+R1H=indene+H2 1.8E13 0.0 0.0 !Est.C5H7#Y+R1H=C5H6#+H2
indanyl-Y+R2OH=indene+H2O 6.0E12 0.0 0.0 !Est.C5H7#Y+R2OH=C5H6#+H2O
indanyl-Y+indanyl-Y=indene+indane 5.0E12 0.0 0.0 !Est.
indanyl-Y+indenyl=2indene 5.0E12 0.0 0.0 !Est.

!**oxidation

indanyl-Y+O2=indene+R3OOH 1.58E12 0.0 15.2E3 !Est.!similar to C5H7#Y+O2=C5H6#+R3OOH A*2

!**isomerization

indanyl-1=indanyl-Y 1.95E10 1.0 34.2E3 !Est.!similar to ph#C4H8-3=ph#C4H8X

!*****!

!* Reactions of C9H9O# (C6H4#CH(O.)/CH2/CH2) *!
!* C9H8O# (C6H4#C(/O)/CH2/CH2) *!
!*****!

C9H9O#=C9H8O#+R1H 9.77E12 0.0 17.3E3 !Est.CH2//CH/CH(O.)/CH3 = H+CH2//CHC(/O)/CH3
C9H9O#=>C6H6#+B2CO+R10C2H3V 2.8E13 0.0 17.1E3 !Est.CH3CO=CH3+CO
C9H9O#=styrene+R5CHO 2.8E13 0.0 17.1E3 !Est.CH3CO=CH3+CO

!*****!
!* Reactions of C2H3C6H4CH2 *!
!* C2H3C6H4CH2O CH2(O.)/C6H4#/CH//CH2 *!
!*****!

!**combinations

C2H3C6H4CH2+R1H=CH3styre 1.0E14 0.0 0.0 !Est. similar to C5H7Y+R1H=C5H8
!C2H3C6H4CH2+R4CH3=C2H3C6H4C2H5 1.5E13 0.0 0.0 ! Est.similar to benzyl+CH3=etC6H5

!**reactions with O2

C2H3C6H4CH2+O2=C2H3C6H4CH2O+B1O 6.3E12 0.0 40.0E3 ! Est.similar to o-methylbenzyl+O2=CH3C6H4CH2O+O

!**termination reactions

C2H3C6H4CH2+B1O=C6H5C2H2+HCHO 3.5E13 0.0 0.0 !Est.similar to o-methylbenzyl+O=C6H4CH3+HCHO
C2H3C6H4CH2+B1O=C2H3C6H4CHO+R1H 1.0E14 0.0 0.0 !Est.similar to o-methylbenzyl+O=CH3C6H4CHO+H
!C2H3C6H4CH2+R2OH=C2H3C6H4CH2OH 2.0E13 0.0 0.0 !Est.similar to o-methylbenzyl+OH=CH3C6H4CH2OH
C2H3C6H4CH2+R3OOH=C2H3C6H4CH2O+R2OH 5.0E12 0.0 0.0 !Est.similar to o-methylbenzyl+OOH=CH3C6H4CH2OOH

!*****!
!* Reactions of C2H3C6H4CH2O CH2(O.)/C6H4#/CH//CH2 *!
!*****!

!**decomposition by beta-scission

C2H3C6H4CH2O=R1H+C2H3C6H4CHO 2.0E13 0.0 27.5E3 !Est.similar to CH3C6H4CH2O=H+CH3C6H4CHO
C2H3C6H4CH2O=C6H5C2H2+HCHO 2.0E13 0.0 27.5E3 !Est.similar to CH3C6H4CH2O=C6H4CH3+HCHO

!**reactions with oxygen

C2H3C6H4CH2O+O2=R3OOH+C2H3C6H4CHO 6.0E10 0.0 1.6E3 !Est.similar to CH3C6H4CH2O+O2=OOH+CH3C6H4CHO

!*****!
!* Reactions of indanyl-1 c(#1)&c(#2)&ch&ch&ch&ch&1,1/CH2/CH(/)/CH2/2 *!
!*****!

!**decomposition by beta-scission

indanyl-1=indene+R1H 6.57E10 0.885 35.77E3 !cal.
indanyl-1=C3H5C6H4 1.11E13 0.150 45.87E3 !cal.

!**oxidation

indanyl-1+O2=indene+R3OOH 3.16E12 0.0 5.0E3 !Est.!similar to ph#C4H8-3+O2=ph#C4H7-2+R3OOH A*2

!*****!

!* Reactions of ph#C3H6-1 (C6H5#/CH2/CH2/CH2(.)) *!

!* ph#C3H6-2 (C6H5#/CH2/CH(.)/CH3) *!

!* ph#C3H6-Y (C6H5#/CH(.)/CH2/CH3) *!

!*****!

!**decomposition by beta-scission

ph#C3H6-1=benzyl+C2H4Z 3.3E13 0.0 22.5E3 !nBB!

ph#C3H6-1=ph#C3H5Z+R1H 3.0E13 0.0 38.0E3 !nBB!

ph#C3H6-2=C6H5#+C3H6Y 2.0E13 0.0 34.5E3 !ph#C4H8-3=C6H5#+C4H8Y

ph#C3H6-2=ph#C3H5p+R1H 3.2E13 0.0 34.8E3 !ph#C4H8-3=ph#C4H7-3+R1H

ph#C3H6-2=ph#C3H5Z+R1H 3.0E13 0.0 38.0E3 !ph#C4H8-3=ph#C4H7-2+R1H

ph#C3H6-Y=R1H+ph#C3H5p 3.0E13 0.0 50.5E3 !C5H9Y=R1H+C5H8

ph#C3H6-Y=styrene+R4CH3 1.3E13 0.0 35.9E3 !ph#C4H8X=styrene+R11C2H5

!**isomerization

ph#C3H6-2=ph#C3H6-Y 1.95E10 1.0 34.2E3 !ph#C4H8-3=ph#C4H8X

ph#C3H6-2=ph#C3H6-1 1.95E10 1.0 38.7E3 !ph#C4H8-3=ph#C4H8-2

ph#C3H6-1=ph#C3H6-Y 3.4E09 1.0 32.5E3 !ph#C4H8-2=ph#C4H8X

!**oxidations

ph#C3H6-1+O2=ph#C3H5Z+R3OOH 1.58E12 0.0 5.0E3 !nBB!

ph#C3H6-2+O2=ph#C3H5p+R3OOH 2.60E11 0.0 2.5E3 !ph#C4H8-3+O2=ph#C4H7-3+R3OOH

ph#C3H6-2+O2=ph#C3H5Z+R3OOH 1.58E12 0.0 5.0E3 !ph#C4H8-3+O2=ph#C4H7-2+R3OOH

ph#C3H6-Y+O2=ph#C3H5p+R3OOH 1.58E12 0.0 15.2E3 !ph#C4H8X+O2=ph#C4H7-3+R3OOH

!**terminaisons

ph#C3H6-Y+R1H=ph#C3H7 1.0E14 0.0 0.0 !

!*****!

!* Reactions of CH3C6H4C3H6 (CH3/C6H4#/CH2/CH2/CH2.) *!

!*****!

!**decomposition by beta-scission

CH3C6H4C3H6=o-methylbenzyl+C2H4Z 3.3E13 0.0 22.5E3 !Est. ph#C3H6-1=benzyl+C2H4Z in nBB!

!*****!

!* Reactions of C3H5C6H4 CH2//CH/CH2/C6H4#(.) *!

!*****!

!C3H5C6H4+R1H=ph#C3H5Z 1.0E14 0.0 0.0 !Est. C6H4#CH3+R1H=toluene!

C3H5C6H4+O2=C3H5C6H4O+B10 2.6E13 0.0 6.1E3 !Est. C6H4#CH3+O2=OC6H4CH3+B10!

!C3H5C6H4+B10=C3H5C6H4O 1.0E14 0.0 0.0 !Est. C6H4#CH3+B10=OC6H4CH3

!C3H5C6H4+R3OOH=C3H5C6H4O+R2OH 5.0E12 0.0 0.0 !Est. C6H4#CH3+HO2=OC6H4CH3+R2OH!

C3H5C6H4=ph#C3H4Y 3.4E13 0.0 34.5E3!Est. C5H7-1s=C5H7Y!

!*****!
!* Reactions of C3H5C6H4O CH2//CH/CH2/C6H4#/O. *!
!*****!

C3H5C6H4O=>C6H6#+B2CO+R10C2H3V 3.0E11 0.0 43.8E3 !Est. OC6H4CH3=>R1H+C6H6#+B2CO!
C3H5C6H4O=>C2H2+B2CO+C4H4+R10C2H3V 3.0E11 0.0 43.8E3 !Est.
OC6H4CH3=>C2H2+C4H4+R1H+B2CO!
C3H5C6H4O=>C3H3+lC5H6+B2CO 1.5E11 0.0 43.8E3 !Est. OC6H4CH3=>C3H3+aC3H4+B2CO

!*****!
!* ph#C3H4Y C6H5#/CH()/CH//CH2 *!
!*****!

ph#C3H4-1=ph#C3H4Y 3.4E13 0.0 34.5E3 !C5H7-1s=C5H7Y
ph#C3H4-2=ph#C3H4Y 1.3E13 0.0 44.5E3 !C5H7-2s=C5H7Y
ph#C3H4-3=ph#C3H4Y 5.0E13 0.0 37.0E3 !C5H7-3t=C5H7Y
ph#C3H4-4=ph#C3H4Y 2.0E13 0.0 47.0E3 !C5H7-4s=C5H7Y

!ph#C3H4-1=C6H5C3H3+R1H 1.5E13 0.0 46.0E3 !Touchard nBB!
!ph#C3H4-2=C6H5C3H3+R1H 1.5E13 0.0 46.0E3 !Touchard nBB!

ph#C3H4-1=benzyl+C2H2 2.0E13 0.0 30.0E3 !C5H7-1s=C2H2+C3H5Y
ph#C3H4-2=C6H5#+aC3H4 2.0E13 0.0 35.5E3 !C5H7-2s=R10C2H3V+aC3H4
ph#C3H4-3=>C6H5#C2H+R4CH3 2.0E13 0.0 31.5E3 !C5H7-3t=R4CH3+C4H4
ph#C3H4-4=>C6H5#+pC3H4 2.0E13 0.0 31.0E3 !C5H7-4s=R10C2H3V+pC3H4

ph#C3H4Y+R1H=ph#C3H5Z 5.0E13 0.0 0.0E3 !Allara80 (touchard)! nBB ! A/2
ph#C3H4Y+R1H=ph#C3H5p 5.0E13 0.0 0.0E3 !Est.! A/2
ph#C3H4Y+R4CH3=ph#C4H7-3 5.0E12 0.0 0.0 !Kingas 1500K

ph#C3H4Y+R3OOH=>R2OH+R10C2H3V+C6H5CHO 5.0E12 0.0 0.0E3 !nBB!
ph#C3H4Y=>C5H5#+C4H4 6.0E13 0.0 70.0E3 !benzyl=>C5H5#+C2H2

ph#C3H4Y+B10=C6H5#+C2H3CHO 3.5E13 0.0 0.0 !benzyl+B10=C6H5#+HCHO
ph#C3H4Y+B10=C6H5CHO+R10C2H3V 1.0E14 0.0 0.0 !benzyl+B10=C6H5CHO+R1H

!*****!
!*****!
!** Second Mechanism **!
!*****!
!*****!

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

!indene+R2OH=>C2H4Z+C6H5CO 1.37E12 0.0 -1.04E3 !nBB!
!indene+R2OH=>R10C2H3V+B2CO+C6H6# 1.37E12 0.0 -1.04E3 !Est.

!indene+R2OH=>o-methylbenzyl+B2CO 1.37E12 0.0 -1.04E3
!indene+R4CH3=C10H11 9.64E10 0.0 8.0E3 !C5H6#+R4CH3=RMCPY1

!indene+O2=R3OOH+indenyl 1.4E12 0.0 28.08E3 !nBB! A delta H cal.
!indene+B10=indenyl+R2OH 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+R1H=benzyl+C2H2 3.0E14 0.0 23.0E3 !A. Laskin , A. Lifshitz,Proc. Combust. Inst. 27
(1998) 313-320.
!indene+R1H=C6H5#C2H+R4CH3 4.0E14 0.0 23.0E3 !A. Laskin , A. Lifshitz,Proc. Combust. Inst. 27
(1998) 313-320.
!indene+R1H=C6H6#+C3H3 2.0E14 0.0 24.5E3 !A. Laskin , A. Lifshitz,Proc. Combust. Inst. 27
(1998) 313-320.
!indene+R2OH=indenyl+H2O 6.0E6 2.0 -1.52E3 !A-I-21 secondary A*2
!indene+R2OH=benzyl+CH2COZ 1.0E13 0.0 5.0E3 !Slavinskaya09
!indene+R4CH3=indenyl+CH4 2.0E11 0.0 7.3E3 !A-I-21 secondary A*2
!indene+R3OOH=H2O2+indenyl 1.28E4 2.6 12.4E3 !A-I-21 secondary A*2

indene+R1H=ph#C3H4Y 5.8E13 0.0 8.1E3 !lipso-addition
indene+R1H=ph#C3H4-1 5.8E13 0.0 8.1E3 !lipso-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 !nBB!
!C6H5#+C3H3=indene 6.46E12 0.0 0.0 !Slavinskaya09
indenyl+R4CH3=methylindene 1.5E13 0.0 0.0 !nBB!
indenyl+R3OOH=C9H7O#+R2OH 3.0E12 0.0 0.0 !Est.!similar to C5H5#+HO2
indenyl+B10=C9H7O# 5.8E13 -0.02 0.02E3 !Est. C5H5#+B10=C5H4O#+R1H
!indenyl+R2OH=>styrene+B2CO 4.0E14 0.0 4.5E3 !Est. C5H5#+OH=C4H6Z2+CO

C9H7O#=C9H6O#+R1H 2.0E13 0.0 27.5E3 ! Est.like ph#CH2O
C9H7O#=>C6H6#+B2CO+R9C2H 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+CO
C9H7O#=>C6H5#C2H+R5CHO 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+CO

!*****!
!*Reactions of methylindane and derived radicals!
!*C10H11 C(#1)&C(#2)&ch&ch&ch&ch&1,1/ch(/ch3)/ch2/ch(./)/2
!*C10H11-1 c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch3)/ch(./)/ch2/2
!*C10H11-2 c(#1)&c(#2)&ch&ch&ch&ch&1,1/ch(/ch2(./))/ch2/ch2/2
!*C10H11-3 c(#1)&c(#2)&ch&ch&ch&ch&1,1/c(./)(/ch3)/ch2/ch2/2
!*****!

!methylindane+R1H=>ph#C4H8-2 5.8E13 0.0 8.1E3 !lipso-addition
methylindane+R1H=>benzyl+C3H6Y 5.8E13 0.0 8.1E3 !lipso-addition
!methylindane+R1H=indane+R4CH3 5.8E13 0.0 8.1E3 !lipso-addition
methylindane+R1H=>C2H4Z+C8H9# 5.8E13 0.0 8.1E3 !lipso-addition

methylindane+R1H=C10H11+H2 5.0E4 2.5 -1.9E3 !Est.similar to MCP+R1H=RMCPY1+H2
methylindane+R1H=C10H11-1+H2 9.0E6 2.0 5.0E3 !Est.similar to MCP+R1H=RMCP1+H2
methylindane+R1H=C10H11-2+H2 2.9E7 2.0 7.7E3 !Est.similar to MCP+R1H=RMCP2+H2
methylindane+R1H=C10H11-3+H2 2.5E4 2.5 -2.79E3 !Est.similar to MCP+R1H=RMCPY2+H2

methylindane+R2OH=C10H11+H2O 3.0E6 2.0 -1.52E3 !Est.similar to MCP+R2OH=RMCPY1+H2O
methylindane+R2OH=C10H11-1+H2O 2.6E6 2.0 -0.77E3 !Est.similar to MCP+R2OH=RMCP1+H2O

methylindane+R2OH=C10H11-2+H2O 2.7E6 2.0 0.45E3 !Est.similar to MCP+R2OH=RMCP2+H2O
methylindane+R2OH=C10H11-3+H2O 1.3E6 2.0 -2.62E3 !Est.similar to MCP+R2OH=RMCPY2+H2O

C10H11-1=C10H11 1.95E10 1.0 34.2E3 !ph#C4H8-3=ph#C4H8X
C10H11=methylindene+R1H 1.21E11 0.985 42.2E3 !C9H9#-1=indene+R1H
C10H11-1=R4CH3+indene 2.0E13 0.0 31.0E3 !Est.similar to RMCP1=R4CH3+C5H6#

C10H11+O2=R3OOH+methylindene 1.58E12 0.0 15.2E3 !Est.similar to RMCPY1+O2=MCPD+R3OOH
C10H11-1+O2=R3OOH+methylindene 2.6E11 0.0 2.5E3 !Est.similar to RMCP1+O2=MCPD+R3OOH
C10H11-1+O2=R3OOH+methylindene-2 2.6E11 0.0 2.5E3 !Est.similar to
RMCP1+O2=MCPD+R3OOH
C10H11-3+O2=R3OOH+methylindene-2 1.58E12 0.0 15.2E3 !Est.similar to
RMCPY1+O2=MCPD+R3OOH

C10H11+R1H=methylindane 1.0E14 0.0 0.0 !Est.similar to RMCPY1+R1H=MCP
C10H11-2=>C6H5C2H2+C2H4Z 2.0E13 0.0 28.7E3 !Est.similar to RMCP2=C2H4Z+nC4H5
C10H11-3+R1H=methylindane 1.0E14 0.0 0.0 !Est.similar to RMCPY2+R1H=MCP

C10H11-3=methylindene-2+R1H 1.21E11 0.985 42.2E3 !C9H9#-1=indene+R1H
C10H11-3=C3H5C6H4CH2 1.36E12 0.44 41.33E3 !C9H9#-1=C2H3C6H4CH2
C3H5C6H4CH2+R1H=C3H5C6H4CH3 1.0E14 0.0 0.0

!*****!

!*Reactions of methylindene!

!*****!

methylindene+B10=>C6H5C2H2+C2H2+R2OH 5.1E13 0.0 7.85E3
methylindene+B10=naphthalene+R1H+R2OH 5.1E13 0.0 7.85E3 !A-I-19 primary A*3
methylindene-2+B10=>naphthalene+R1H+R2OH 5.1E13 0.0 7.85E3 !A-I-19 primary A*3
methylindene+R1H=>C6H5C2H2+C2H2+H2 2.85E7 2.0 7.7E3 !
methylindene+R1H=naphthalene+R1H+H2 2.85E7 2.0 7.7E3 !
methylindene-2+R1H=naphthalene+R1H+H2 2.85E7 2.0 7.7E3 !
methylindene+R2OH=>C6H5C2H2+C2H2+H2O 2.67E6 2.0 0.45E3 !
methylindene+R2OH=naphthalene+R1H+H2O 2.67E6 2.0 0.45E3 !
methylindene-2+R2OH=naphthalene+R1H+H2O 2.67E6 2.0 0.45E3 !
methylindene+R4CH3=>C6H5C2H2+C2H2+CH4 3.0E-1 4.0 8.2E3 !
methylindene+R4CH3=naphthalene+R1H+CH4 3.0E-1 4.0 8.2E3 !
methylindene-2+R4CH3=naphthalene+R1H+CH4 3.0E-1 4.0 8.2E3 !

!methylindene+R1H=C10H11 2.6E13 0.0 3.2E3 !Est. MCPD+R1H=RMCP1
methylindene+R1H=C10H11-1 2.6E13 0.0 3.2E3 !Est. MCPD+R1H=RMCPY1

methylindene+R1H=>C2H2+C8H9# 5.8E13 0.0 8.1E3 !ipso-addition

!*****!

!*Reactions of C9H8O# !! C6H4#/C(//O)/CH2/CH2/ *!

!*****!

C9H8O#+R1H=>styrene+R1H+B2CO 5.8E13 0.0 8.1E3 !similar to ipso-addition reaction !
C9H8O#+B10=styrene+CO2 1.0E13 0.0 2.0E3 !Est.Alzueta C5H4O#
!C9H8O#+B10=styrene+CO2 1.2E11 0.7 8.96E3 !Est.Touchard A-I-20 secondaire
!C9H8O#+B10=styrene+CO2 1.0E13 0.0 2.0E3 !Est.similar to C5H4O#+B10=C4H4+CO2!

!*****!
!* Reactions of C9H6O# and derived radicals !! *!
!*****!

C9H6O#+R1H=>C6H5#C2H+R1H+B2CO 5.8E13 0.0 8.1E3 !ipso-addition?
C9H6O#+B10=C6H5#C2H+CO2 1.0E13 0.0 2.0E3 !Est.Alzueta C5H4O#
!C9H6O#+B10=C6H5#C2H+CO2 6.0E10 0.7 8.96E3 !Est.Touchard A-I-20 secondaire
!C9H6O#+B10=C6H5#C2H+CO2 1.0E13 0.0 2.0E3 !Est.similar to C5H4O#+B10=C4H4+CO2

!*****!
!* Reactions of naphthalene *!
!*****!

!2C5H5#=naphthalene+H2 4.3E36 -6.3 22.835E3 !in Slavinskaya09, A.M. Dean, J. Phys. Chem. 94 (1990) 1432-1439.
!C6H5#+iC4H3=naphthalene 3.18E23 -3.2 2.13E3 !in Slavinskaya09, H.Y. Zhang, J.T. McKinnon, CST 107 (1995) 261-300.
!C6H5#+iC4H3=naphthyl+R1H 2.0E-10 7.1 0.786E3 !in Slavinskaya09, H.Y. Zhang, J.T. McKinnon, CST 107 (1995) 261-300.
!C6H5#+C4H4=naphthalene+R1H 3.3E33 -5.7 12.75E3 !in Slavinskaya09, J. Appel, H. Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
!benzyl+C3H3=naphthalene+R1H+R1H 6.0E11 0.0 0.0 !in Slavinskaya09, M.B. Colket, D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
!C6H5C2H2+C2H2=naphthalene+R1H 1.6E16 -1.33 3.3E3 !in Slavinskaya09, J. Appel, H. Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.

!naphthalene+O2=R3OOH+naphthyl 8.0E13 0.0 63.4E3 !nBB?!
!naphthalene+B10=>indenyl+B2CO+R1H 2.7E13 0.0 3.6E3 !nBB?!
!naphthalene+R1H=naphthyl+H2 8.0E8 1.8 16.8E3 !nBB?!
!naphthalene+B10=naphthyl+R2OH 2.7E13 0.0 14.7E3 !nBB?!
!naphthalene+R2OH=naphthyl+H2O 2.1E8 1.42 1.45E3 !nBB?!
!naphthalene+R3OOH=naphthyl+H2O2 7.3E12 0.0 28.9E3 !nBB?!
!naphthalene+R4CH3=naphthyl+CH4 2.7E12 0.0 15.0E3 !nBB?!
naphthalene+R9C2H=A2C2H+R1H 5.0E13 0.0 0.0 !in Slavinskaya09, J. Appel, H. Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
naphthalene+B5CH2=A2CH3 2.2E13 0.0 8.63E3 !in Slavinskaya09 modif Ea
naphthalene+B6CH2=A2CH3 4.4E13 0.0 8.68E3 !in Slavinskaya09 modif Ea

!naphthyl+R1H=naphthalene 1.0E14 0.0 0.0E3 !nBB?!
!naphthyl+O2=>indenyl+B2CO+B10 2.6E13 0.0 6.1E3 !nBB?!
!naphthyl+B10=>indenyl+B2CO 1.0E14 0.0 0.0 !nBB?!
!naphthyl+R3OOH=>indenyl+B2CO+R2OH 5.0E12 0.0 0.0 !nBB?!
!naphthyl+R2OH=>indenyl+B2CO+R1H 1.0E13 0.0 0.0 !nBB?!
naphthyl+C2H2=A2C2H+R1H 1.3E24 -3.06 22.45E3 !in 09, J. Appel, H. Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.modif Ea

!naphthyl+C2H2=>A2R5+R1H 1.0E13 0.0 0.0! Roda
naphthyl+C2H2=A2R5+R1H 1.9E31 -5.26 20.86E3!in Slavinskaya09 modif Ea

A2C2H+R1H=A2R5+R1H 4.6E37 -7.03 22.95E3 !in Slavinskaya09 modif Ea
!A2R5=C6H5#C2H+C4H2 1.0E10 0.0 79.48E3 !in Slavinskaya09 modif Ea

A2C2H+R2OH=naphthyl+CH2COZ 2.18E-4 4.5 -993.5 !in Slavinskaya09, J. Appel, H. Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.modif Ea
indenyl+C3H3=>A2C2H+2R1H 6.0E11 0.0 0.0 !in Slavinskaya09, M.B. Colket, D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.

A2CH3=naphthyl+R4CH3 1.0E16 0.0 96.97E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3=A2CH2+R1H 2.81E15 0.0 88.82E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+O2=A2CH2+R3OOH 3.0E14 0.0 41.35E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+B1O=A2CH2+R2OH 1.2E13 0.0 1.29E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+R1H=A2CH2+H2 3.98E2 3.44 3.1E3 !in Slavinskaya09, M.S. Skjoth-Rasmussen, P. Glarborg, M. Ostberg, J.T. Johannessen, H. Livbjerg, A.D. Jensen, T.S. Christensen, CaF 136 (2004) 91-128.modif Ea
A2CH3+R1H=naphthalene+R4CH3 1.2E13 0.0 5.07E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+R2OH=A2CH2+H2O 5.19E8 1.0 0.87E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+R3OOH=A2CH2+H2O2 4.0E11 0.0 13.91E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea
A2CH3+R4CH3=A2CH2+CH4 1.58E12 0.0 10.93E3 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.modif Ea

A2CH2+B1O=naphthyl+HCHO 1.65E14 0.0 0.0 !in Slavinskaya09, H. Pitsch, Proc. Combust. Inst. 26 (1996) 721-728.
A2CH2+R3OOH=>naphthyl+HCHO+R2OH 1.0E13 0.0 0.0 !in Slavinskaya09, M.S. Skjoth-Rasmussen, P. Glarborg, M. Ostberg, J.T. Johannessen, H. Livbjerg, A.D. Jensen, T.S. Christensen, CaF 136 (2004) 91-128.
A2CH2+B5CH2=A2C2H+H2+R1H 2.4E14 0.0 0.0 !in Slavinskaya09
A2CH2+C3H3=>phenanthrene+2R1H 5.0E12 0.0 0.0 !in Slavinskaya09
!C6H5#C2H+C6H5#=phenanthrene+R1H 1.1E23 -2.92 15.92E3 !in Slavinskaya09 modif Ea
!indenyl+C5H5#=phenanthrene+2R1H 4.3E13 0.0 9.72E3 !in Slavinskaya09 A/10 modif Ea A*10

phenanthrene=>naphthalene+C4H2 1.0E11 0.0 89.42E3 !in Slavinskaya09 A/10 modif Ea A*10
phenanthrene=A2R5+C2H2 2.0E11 0.0 89.42E3 !in Slavinskaya09 A/10 modif Ea A*10
phenanthrene+B1O=A2C2H+CH2COZ 2.2E13 0.0 5.49E3 !in Slavinskaya09, H.Wang, M. Frenklach, Combust. Flame 110 (1997) 173-221.modif Ea
phenanthrene+R2OH=>A2C2H+CH2COZ+R1H 1.3E13 0.0 9.94E3 !in Slavinskaya09, H.Wang, M. Frenklach, Combust. Flame 110 (1997) 173-221.modif Ea

phenanthrene+B5CH2=CH3phenanth 2.2E13 0.0 7.16E3 !in Slavinskaya09, H. Kraus, C. Oehlers, F. Temps, H.G. Wagner, J. Phys. Chem. 97 (1993) 10989-10995.modif Ea
phenanthrene+B6CH2=CH3phenanth 4.2E13 0.0 7.166E3 !in Slavinskaya09, H. Kraus, C. Oehlers, F. Temps, H.G. Wagner, J. Phys. Chem. 97 (1993) 10989-10995.modif Ea
antra=phenanthrene 7.940E+12 0.00 65000.00 !Marinov!

CH3phenanth=>CH2phenanth+R1H 2.81E15 0.0 88.82E3 !in Slavinskaya09 modif Ea
CH3phenanth+O2=CH2phenanth+R3OOH 3.0E14 0.0 41.35E3 !in Slavinskaya09 modif Ea
CH3phenanth+B1O=CH2phenanth+R2OH 1.2E13 0.0 1.28E3 !in Slavinskaya09 modif Ea
CH3phenanth+R1H=phenanthrene+R4CH3 1.2E13 0.0 5.07E3 !in Slavinskaya09, modif Ea
CH3phenanth+R1H=CH2phenanth+H2 1.2E14 0.0 8.35E3 !in Slavinskaya09, N.M. Marinov, W.J. Pitz, C.K. Westbrook, M.J. Castaldi, S.M. Senkan, CST 116/117 (1996) 211-287 modif Ea

CH3phenanth+R2OH=CH2phenanth+H2O 1.26E13 0.0 2.53E3 !in Slavinskaya09,M.S. Skjoth-Rasmussen, P. Glarborg, M. Ostberg, J.T. Johannessen, H. Livbjerg, A.D. Jensen,T.S. Christensen, CaF 136 (2004)91-128. modif Ea
CH3phenanth+R3OOH=CH2phenanth+H2O2 4.0E11 0.0 13.91E3 !in Slavinskaya09 modif Ea
CH3phenanth+R4CH3=CH2phenanth+CH4 1.58E12 0.0 10.93E3 !in Slavinskaya09 modif Ea

CH2phenanth+B5CH2=pyrene+H2+R1H 2.4E14 0.0 0.0 !in Slavinskaya09

!pyrene=C4H2+A2R5 1.0E11 0.0 89.42E3 !A/10 in Slavinskaya09,A. Laskin , A. Lifshitz,Proc. Combust. Inst. 27 (1998) 313-320 modif Ea A*10
naphthyl+C6H6#=pyrene+R1H+H2 1.0E12 0.0 4.97E3 !in Slavinskaya09,M.B. Colket, D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891. modif Ea
naphthyl+C6H5#=>pyrene+H2 4.3E37 -6.3 44.87E3 !in Slavinskaya09 modif Ea

!A2CH2+C6H5#=chrysene+2R1H 1.1E24 -2.92 15.92E3 !in Slavinskaya09 modif Ea
chrysene=>C4H2+phenanthrene 1.0E11 0.0 89.42E3 !in Slavinskaya09 A/10 modif Ea A*10
chrysene=C2H2+pyrene 1.0E11 0.0 89.42E3 !in Slavinskaya09 A/10 modif Ea A*10

!naphthyl+O2=A2O+B1O 2.6E13 0.0 6.1E3 !<estimated(f)>!Roda
!naphthyl+B1O=A2O 1.0E14 0.0 0.0 !<estimated(f)>!Roda
naphthyl+R2OH=naphtol 1.0E13 0.0 0.0 !<estimated(f)>!Roda
!naphthyl+R3OOH=A2O+R2OH 5.0E12 0.0 0.0 !<estimated(f)>!Roda
!naphthyl+R2OH=A2O+R1H 5.0E12 0.0 0.0 !<estimated(f)>! ** AJOUT Roda

!*****!
!* REACTIONS OF naphthol AND DERIVED RADICALS *! comme le phenol
!*****!

!naphthol+O2=R3OOH+A2O 1.0E13 0.0 38.9E3 !<ALZUETA00>!
!naphthol+R1H= naphthalene + R2OH 2.23E13 0.0 7.95E3
naphthol+R1H = A2O+H2 1.2E14 0.0 12.4E3 !<ALZUETA00>!
naphthol+B1O = A2O+R2OH 1.3E13 0.0 2.9E3 !<ALZUETA00>!
naphthol+R2OH = A2O+H2O 1.4E8 1.4 -0.96E3 !<SHANDROSS96>!
naphthol+R3OOH = A2O+H2O2 1.0E12 0.0 10.0E3 !<ALZUETA00>!
naphthol+R4CH3 = A2O+CH4 1.8E11 0.0 7.7E3 !<MULCAHY65>!

!*****!
!* REACTIONS OF A2O RADICALS *!
!*****!

!**CO elimination with rearrangement
!A2O=indenyl+B2CO 3.0E11 0.0 43.8E3!<FRANCK94>!Roda

!**termination reactions!
A2O+R1H=naphtol 1.0E14 0.0 0.0E3 !<estimated(g)>!Roda

!*****!
!*Reactions of C3H5C6H4CH3 CH2//CH/CH2/C6H4/CH3 !
!*****!

C3H5C6H4CH3+R1H=toluene+C3H5Y 5.8E13 0.0 8.1E3 !ipso-addition

C3H5C6H4CH3+R1H=ph#C3H5Z+R4CH3 5.8E13 0.0 8.1E3 !ipso-addition

!*****!

!* Reactions of CH3C6H4C3H7 (CH3/C6H4#/CH2/CH2/CH3) *!

!*****!

!CH3C6H4C3H7+R1H=toluene+nC3H7 5.8E13 0.0 8.1E3 !ipso-addition

!CH3C6H4C3H7+R1H=ph#C3H7+R4CH3 5.8E13 0.0 8.1E3 !ipso-addition

!*****!

!* Reactions of ph#C3H5Z (C6H5#CH2/CH//CH2) !!!

!*****!

!Unimolecular initiation

!benzyl+R10C2H3V=ph#C3H5Z 1.5E13 0.0 0.0 !benzyl+R11C2H5=ph#C3H7

!C6H5#+C3H5Y=ph#C3H5Z 1.5E13 0.0 0.0 !C6H5#+nC3H7=ph#C3H7

!**bimolecular initiation (DH 1200K)!

!ph#C3H5Z+O2=ph#C3H4Y+R3OOH 1.4E11 0.0 26.31E3 !as Ingham & Walker! nBB !

!**addition-decomposition

ph#C3H5Z+B10=>benzyl+R13CH2CHO 6.40E04 2.56 -1.13E3 !Touchard! nBB !

ph#C3H5Z+R2OH=>HCHO+C8H9#-1 1.37E12 0.0 -1.04E3 !nBB !

ph#C3H5Z+R4CH3=>benzyl+C3H6Y 1.69E11 0.0 7.40E3 !nBB !

!**ipso-additions

ph#C3H5Z+R4CH3=>toluene+C3H5Y 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene)! nBB !A*1

ph#C3H5Z+R1H=>C6H6#+C3H5Y 5.8E13 0.0 8.1E3 !ipso-addition

!**Metatheses

ph#C3H5Z+B10=ph#C3H4Y+R2OH 8.8E10 0.7 3.25E3 !Buda! nBB !

ph#C3H5Z+R1H=ph#C3H4Y+H2 5.4E04 2.5 -1.9E3 ! Table A-I-21 H secondary A*2

ph#C3H5Z+R2OH=ph#C3H4Y+H2O 3.0E06 2.0 -1.52E3 ! Table A-I-21 H secondary A*2

ph#C3H5Z+R4CH3=ph#C3H4Y+CH4 1.0E11 0.0 7.30E3 !nBB !

ph#C3H5Z+R3OOH=ph#C3H4Y+H2O2 6.4E3 2.6 12.4E3 ! Table A-I-21 H secondary A*2

!*****!

!* Reactions of ph#C3H5p (C6H5#CH//CH/CH3) !!!

!*****!

!Unimolecular initiation

!benzyl+R10C2H3V=ph#C3H5p 1.5E13 0.0 0.0 !benzyl+R11C2H5=ph#C3H7

!C6H5#+C3H5Y=ph#C3H5p 1.5E13 0.0 0.0 !C6H5#+nC3H7=ph#C3H7

ph#C3H5p+R2OH=>benzyl+CH3CHO 1.37E12 0.0 -1.04E3 ! ph#C3H5Z+R2OH

ph#C3H5p+R2OH=>C6H5CHO+R11C2H5 1.37E12 0.0 -1.04E3 ! ph#C3H5Z+R2OH

ph#C3H5p+R1H=>C6H6#+C3H5Y 5.8E13 0.0 8.1E3 !ipso-addition

ph#C3H5p+R4CH3=>toluene+C3H5Y 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene)! nBB !A*1

ph#C3H5p+R4CH3=>benzyl+C3H6Y 1.69E11 0.0 7.40E3

ph#C3H5p+R1H=ph#C3H4Y+H2 5.8E04 2.5 2.51E3 !Table A-I-21 H primary A*1

ph#C3H5p+B10=ph#C3H4Y+R2OH 5.8E10 0.7 5.9E3 !Table A-I-21 H primary A*1
ph#C3H5p+R2OH=H2O+ph#C3H4Y 1.0E6 2.0 -0.298E3 !Table A-I-21 H primary A*1
ph#C3H5p+R4CH3=ph#C3H4Y+CH4 0.74E0 3.5 5.67E3 !Table A-I-21 H primary A*1
ph#C3H5p+R3OOH=ph#C3H4Y+H2O2 3.2E3 2.6 13.9E3 !Table A-I-21 H primary A*1

!*****

!* Reactions of ph#C3H7 (C6H5#CH2/CH2/CH3) !!!

!*****

!Unimolecular initiation

!C8H9#-1+R4CH3=ph#C3H7 1.5E13 0.0 0.0 !Est.nBB!

!benzyl+R11C2H5=ph#C3H7 1.5E13 0.0 0.0 !Est.nBB!

!C6H5#+nC3H7=ph#C3H7 1.5E13 0.0 0.0 !Est.nBB!

!**bimolecular initiation (DH 1200K)

!ph#C3H7+O2=>styrene+R4CH3+R3OOH 1.4E12 0.0 35.11E3 !Touchard and Kingas! nBB!

!ph#C3H7+O2=ph#C3H6-1+R3OOH 2.1E13 0.0 52.29E3 !nBB!

!**ipso-addition

ph#C3H7+R1H=C6H6#+nC3H7 5.8E13 0.0 8.1E3 !<BAULCH94> (Toluene) !nBB!

ph#C3H7+R4CH3=toluene+nC3H7 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene) !nBB! A*1

!**Metatheses

ph#C3H7+R1H=ph#C3H6-Y+H2 5.4E4 2.5 -1.9E3 !ph#C4H9+R1H=ph#C4H8X+H2

ph#C3H7+B10=ph#C3H6-Y+R2OH 8.8E10 0.7 3.25E3 !ph#C4H9+B10=ph#C4H8X+R2OH

ph#C3H7+R2OH=ph#C3H6-Y+H2O 3.0E6 2.0 -1.52E3 !ph#C4H9+R2OH=ph#C4H8X+H2O

ph#C3H7+R3OOH=ph#C3H6-Y+H2O2 6.4E03 2.6 12.4E3 !ph#C4H9+R3OOH=ph#C4H8X+H2O2

ph#C3H7+R4CH3=ph#C3H6-Y+CH4 1.0E11 0.0 7.3E3 !ph#C4H9+R4CH3=ph#C4H8X+CH4

!*****

!* Reactions of ph#C4H9 (C6H5#CH2/CH2/CH2/CH3) !!!

!* ph#C4H8-X (C6H5#/CH./CH2/CH2/CH3) !

!*****

!**IPSO-ADDITIONS

ph#C4H9+R1H=C6H6#+R20C4H9 5.8E13 0.0 8.1E3 !<BAULCH94>(Toluene and ethylbenzene)!BBZ

ph#C4H9+R4CH3=toluene+R20C4H9 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene)!BBZ

!**METATHESSES

ph#C4H9+R1H=ph#C4H8X+H2 5.4E4 2.5 -1.9E3 !<BUDA> (Touchard)!

ph#C4H9+B10=ph#C4H8X+R2OH 8.8E10 0.7 3.25E3 !<BUDA>(Touchard,Table A-I-21)!

ph#C4H9+R2OH=ph#C4H8X+H2O 3.0E6 2.0 -1.52E3 !<BUDA> (Touchard)!

ph#C4H9+R3OOH=ph#C4H8X+H2O2 6.4E03 2.6 12.4E3 !<BUDA> (Touchard)!

ph#C4H9+R4CH3=ph#C4H8X+CH4 1.0E11 0.0 7.3E3 !<BUDA> (Touchard)!

!**DECOMPOSITION BY BETA-SCISSION

ph#C4H8X=styrene+R11C2H5 1.3E13 0.0 35.9E3 !<Perrin88> (Touchard)!

!COMBINATIONS WITH H

ph#C4H8X+R1H=ph#C4H9 1.0E14 0.0 0.0 !<Allara80>(Touchard)!

!CASSURE LIAISON C-C

!ph#C4H9=C6H5#+R20C4H9 1.00E16 0.0 97.00E3 !<RAO>(Toluene)!

!ph#C4H9=benzyl+nC3H7 2.45E16 0.0 74.71E3 !x10(Kingas at 1200 K)!

!ph#C4H9=C8H9#-1+R11C2H5 3.23E15 0.0 84.10E3 !<Estimated>(Kingas at 1200 K)!

!ph#C4H9=ph#C3H6-1+R4CH3 1.67E16 0.0 86.63E3 !nBB!

!COMBINATIONS WITH H

!ph#C4H8-3+R1H=ph#C4H9 1.0E14 0.0 0.0

!ph#C4H8-3=ph#C3H5Z+R4CH3 2.0E13 0.0 32.5E3 !<Tsang91>(Touchard)!

!ph#C4H8-2+R1H=ph#C4H9 1.0E14 0.0 0.0

!ph#C4H8-2=benzyl+C3H6Y 3.3E13 0.0 22.5E3 !<GIERCZAK86>(Touchard)!

!ph#C4H7-2+R1H=C6H6#+C4H7Y 5.8E13 0.0 8.1E3 !<BAULCH94>(Toluene)!

!ph#C4H7-2+R4CH3=toluene+C4H7Y 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene)

!ph#C4H7-3+R1H=C6H6#+C4H7Y 5.8E13 0.0 8.1E3 !<BAULCH94>(Toluene)!

!ph#C4H7-3+R4CH3=toluene+C4H7Y 1.2E12 0.0 15.9E3 !<Robaugh86>(NIST,Benzene)

!*****

!* Reactions of fulvene

!*****

!C6H6#+R1H=fulvene+R1H 8.43E+32 -4.95 51244.0 !Pitz

!fulvene+R1H=C6H6#+R1H 3.0E12 0.5 2.0E3 !Law07

fulvene+R1H=C6H6#+R1H 3.0E12 0.5 2.0E3 !! Hanson09

!fulvene=C6H6# 2.95E+31 -4.97 88470.0 !PITZ2001

fulvene=C6H6# 5.6234E+81 -19.36 121500. !Hanson09 bpick jul03

!fulvene=C6H5#+R1H 8.51E+24 -2.51 113300.0 !PITZ2001

fulvene=C6H5#+R1H 2.5704E+97 -23.16 153470. !Hanson09 bpick jul03

C3H3+C3H3=fulvene 1.26E+56 -12.61 23520.0 !PITZ2001

!C3H3+C3H3=fulvene 7.25E+65 -16.015 25.035E3 ! Hanson09

!C3H3+C3H3=fulvene 4.19E+39 -8.958 6.098E3 ! Hanson09

C3H3+C3H5Y=>fulvene+2R1H 3.26E29 -5.397 3.39E3 ! JAM, YG, et al 2007 in Hanson09

nC4H3+R10C2H3V=fulvene 4.0E12 0.0 0.0 !in Hanson09

iC4H3+R10C2H3V=fulvene 1.0E13 0.0 0.0 !in Hanson09 JAM6

nC4H5+C2H2=fulvene+R1H 2.52E-9 -0.76 4.412E3 ! in Hanson09

nC4H5+R9C2H=fulvene 4.0E12 0.0 0.0 !in Hanson09

iC4H5+C2H2=fulvene+R1H 6.5E24 -3.44 20.319E3 !in Hanson09

iC4H5+R9C2H=fulvene 1.0E13 0.0 0.0 !in Hanson09

!*****!

!*REACTIONS OF o-xylene MOLECULES*!

!*****!

!**UMIMOLECULAR INITIATIONS

o-xylene = o-methylbenzyl+ R1H 0.5e16 0.0 88.3e3 !<DACOSTA00>! /2
o-xylene=C6H4CH3+R4CH3 4.0E17 0.0 97.0E3 !<COLKET94>*10! *4

!**BIMOLECULAR INITIATION

o-xylene+O2=o-methylbenzyl+R3OOH 4.2E12 0.0 38.6E3 !<estimated(aaa)>*2

!**ADDITIONS

o-xylene+R1H=toluene+R4CH3 11.6E13 0.0 8.1E3 !<BAULCH94>! *2
o-xylene+B1O=OC6H3(CH3)2+R1H 1.7E13 0.0 3.6E3 !<TAPPE89>! *1
o-xylene+R2OH=HOC6H3(CH3)2+R1H 1.3E13 0.0 10.6E3 !<BAULCH94>! *1

!**METATHESES

!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

o-xylene+R1H=o-methylbenzyl+H2 2.4E14 0.0 8.4E3 !<HIPPLER90-1>! *2
o-xylene+B1O=o-methylbenzyl+R2OH 12.6E11 0.0 0.0 !<HOFFMANN90>! *2
o-xylene+R2OH=o-methylbenzyl+H2O 10.4E9 1.0 0.87E3 !<BAULCH94>! *2
o-xylene+R3OOH=o-methylbenzyl+H2O2 8.0E11 0.0 14.0E3 !<BAULCH94>! *2
o-xylene+R4CH3=o-methylbenzyl+CH4 3.2E12 0.0 11.1E3 !<COLKET94>! *2
o-xylene+R10C2H3V=o-methylbenzyl+C2H4Z 8.0e12 0.0 8.0e3 !<COLKET94>! *2

o-xylene+C3H5Y=o-methylbenzyl+C3H6Y 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
o-xylene+C3H3=o-methylbenzyl+pC3H4 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
o-xylene+iC4H5=o-methylbenzyl+C4H6Z2 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
o-xylene+nC4H5=o-methylbenzyl+C4H6Z2 3.2E12 0.0 11.1E3 !<estimated(a)>! *2
o-xylene+C5H5#=o-methylbenzyl+C5H6# 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

o-xylene+C6H5#=o-methylbenzyl+C6H6# 7.9E13 0.0 12.0E3 !<HECKMANN96>! *2
o-xylene+benzyl=o-methylbenzyl+toluene 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

o-xylene+C6H5O#=o-methylbenzyl+C6H5OH# 3.2E11 0.0 15.1E3 !<estimated(a)>! *2
o-xylene+ phenyl(CH3)2=o-methylbenzyl+o-xylene 15.8E13 0.0 12.0E3 !<estimated(b)>! *2
o-xylene+OC6H4CH3=o-methylbenzyl+HOC6H4CH3 3.2E11 0.0 15.1E3 !<estimated(a)>! *2
o-xylene+C6H5CH2OO=o-methylbenzyl+C6H5CH2OOH 8.0E11 0.0 14.0E3 !<estimated(c)>! *2
o-xylene+C6H5CH2O=o-methylbenzyl+C6H5CH2OH 3.2E11 0.0 11.1E3 !<estimated(a)>! *2
o-xylene+HOC6H4CH2=o-methylbenzyl+HOC6H4CH3 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

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

o-xylene+R1H= phenyl(CH3)2+H2 12.0E08 1.0 16.8E3 !<estimated(d)>! *1
o-xylene+B1O= phenyl(CH3)2+R2OH 4.0E13 0.0 14.7E3 !<estimated(d)>! *1
o-xylene+R2OH= phenyl(CH3)2+H2O 3.2E08 1.42 1.45E3 !<estimated(d)>! *1
o-xylene+R3OOH= phenyl(CH3)2+H2O2 11.0E12 0.0 28.9E3 !<estimated(d)>! *1
o-xylene+R4CH3= phenyl(CH3)2+CH4 4.0E12 0.0 15.0E3 !<estimated(d)>! *1

!*****!

!*REACTIONS OF BENZYL HYDROPEROXYDE*!

!*****!

CH3C6H4CH2OOH=CH3C6H4CH2O+R2OH 1.5E16 0.0 42.0E3 !<estimated(r)>! *1

!*****!

!*REACTIONS OF CRESOL AND DERIVED RADICALS*!

!*****!

! amorage

HOC6H3(CH3)2+O2=OC6H3(CH3)2+R3OOH 1.0E13 0.0 38.9E3 !<estimated(s)>!

ralenti *1

HOC6H3(CH3)2+O2=CH3HOC6H3CH2+R3OOH 2.1E12 0.0 38.6E3 !RODA <estimated(aaa)>! *1

! addition

HOC6H3(CH3)2+R1H=HOC6H4CH3+R4CH3 5.8E13 0.0 8.1E3 !<estimated(t)>!

*1

! metatheses

HOC6H3(CH3)2+R1H=OC6H3(CH3)2+H2 1.2E14 0.0 12.4E3 !<estimated(s)>! *1

HOC6H3(CH3)2+B10=OC6H3(CH3)2+R2OH 1.3E13 0.0 2.9E3 !<estimated(s)>! *1

HOC6H3(CH3)2+R2OH=OC6H3(CH3)2+H2O 1.4E8 1.4 -0.96E3

!<estimated(s)>! *1

HOC6H3(CH3)2+R3OOH=OC6H3(CH3)2+H2O2 1.0E12 0.0 10.0E3 !<estimated(s)>! *1

HOC6H3(CH3)2+R4CH3=OC6H3(CH3)2+CH4 1.8E11 0.0 7.7E3 !<estimated(s)>! *1

HOC6H3(CH3)2+C6H5#=OC6H3(CH3)2+C6H6# 4.9E12 0.0 4.4E3 !<estimated(s)>! *1

HOC6H3(CH3)2+C5H5#=OC6H3(CH3)2+C5H6# 4.9E11 0.0 9.4E3 !<estimated(s)>! *1

HOC6H3(CH3)2+C3H5Y=OC6H3(CH3)2+C3H6Y 4.9E11 0.0 9.4E3 !<estimated(s)>! *1

HOC6H3(CH3)2+iC4H5=OC6H3(CH3)2+C4H6Z2 4.9E11 0.0 9.4E3 !<estimated(s)>! *1

HOC6H3(CH3)2+C6H5O#=#OC6H3(CH3)2+C6H5OH# 4.9E11 0.0 9.4E3

!<estimated(s)>! *1

HOC6H3(CH3)2+o-methylbenzyl=OC6H3(CH3)2+o-xylene 4.9E11 0.0 9.4E3

!<estimated(s)>! *1

HOC6H3(CH3)2+R1H=CH3HOC6H3CH2+H2 2.4E14 0.0 8.4E3 !<estimated(t)>! *2

HOC6H3(CH3)2+B10=CH3HOC6H3CH2+R2OH 12.6E11 0.0 0.0

!<estimated(t)>! *2

HOC6H3(CH3)2+R2OH=CH3HOC6H3CH2+H2O 10.4E9 1.0 0.87E3 !<estimated(t)>! *2

HOC6H3(CH3)2+R3OOH=CH3HOC6H3CH2+H2O2 8.0E11 0.0 14.0E3 !<estimated(t)>! *2

HOC6H3(CH3)2+R4CH3=CH3HOC6H3CH2+CH4 3.2E12 0.0 11.1E3 !<estimated(t)>! *2

HOC6H3(CH3)2+C3H5Y=CH3HOC6H3CH2+C3H6Y 3.2E12 0.0 15.1E3

!<estimated(t)>! *2

HOC6H3(CH3)2+C3H3=CH3HOC6H3CH2+pC3H4 3.2E12 0.0 15.1E3

!<estimated(t)>! *2

HOC6H3(CH3)2+iC4H5=CH3HOC6H3CH2+C4H6Z2 3.2E12 0.0 15.1E3

!<estimated(t)>! *2

HOC6H3(CH3)2+nC4H5=CH3HOC6H3CH2+C4H6Z2 3.2E12 0.0 11.1E3 !<estimated(t)>! *2

HOC6H3(CH3)2+C5H5#=CH3HOC6H3CH2+C5H6# 3.2E11 0.0 15.1E3

!<estimated(t)>! *2

HOC6H3(CH3)2+C6H5#=CH3HOC6H3CH2+C6H6# 15.8E13 0.0 12.0E3

!<estimated(t)>! *2

HOC6H3(CH3)2+C6H5O# = CH3HOC6H3CH2+C6H5OH#	3.2E11	0.0	15.1E3	
!<estimated(t)>! *2				
HOC6H3(CH3)2+o-methylbenzyl=CH3HOC6H3CH2+o-xylene	3.2E11	0.0	15.1E3	
!<estimated(t)>! *2				
HOC6H3(CH3)2+C6H4CH3=CH3HOC6H3CH2+toluene	15.8E13	0.0	12.0E3	
!<estimated(t)>! *2				
HOC6H3(CH3)2+OC6H4CH3=CH3HOC6H3CH2+HOC6H4CH3	3.2E11	0.0	15.1E3	
!<estimated(t)>! *2				
HOC6H3(CH3)2+C6H5CH2OO=CH3HOC6H3CH2+C6H5CH2OOH		8.0E11	0.0	14.0E3
!<estimated(t)>! *2				
HOC6H3(CH3)2+C6H5CH2O=CH3HOC6H3CH2+C6H5CH2OH	3.2E11	0.0	11.1E3	
!<estimated(t)>! *2				
CH3HOC6H3CH2+O2=CH3HOC6H3CH2OO	4.6E11	0.0	-377.0	!<estimated(u)>! *1
CH3HOC6H3CH2+O2=CH3HOC6H3CH2O+B1O	6.3E12	0.0	40.0E3	!<estimated(u)>! *1
CH3HOC6H3CH2+R3OOH=CH3HOC6H3CH2O+R2OH	5.0E12	0.0	0.0	
!<estimated(u)>! *1				
CH3HOC6H3CH2+R1H=HOC6H3(CH3)2	1.0E14	0.0	0.0	!<estimated(g)>! *1
CH3HOC6H3CH2+R4CH3=HOC6H4CH3+C2H4Z	5.0E12	0.0	0.0	!<estimated(g)>! *1
CH3HOC6H3CH2OO=CH3OHC6H3CHO+R2OH	3.4E9	1.0	37.5E3	!<estimated(v)>! *1
CH3HOC6H3CH2O=R1H+CH3OHC6H3CHO	2.0E13	0.0	27.5E3	
!<estimated(w)>! *1				
CH3HOC6H3CH2O=CH3C6H4OH#+HCHO	2.0E13	0.0	27.5E3	
!<estimated(w)>! *1				
CH3HOC6H3CH2O+O2=R3OOH+CH3OHC6H3CHO	6.0E10	0.0	1.6E3	!<estimated(w)>! *1
CH3OHC6H3CHO+R1H= CH3C6H3OHCO+H2	4.0E13	0.0	3.2E3	!<estimated(x)>! *1
CH3OHC6H3CHO+B1O= CH3C6H3OHCO+R2OH	6.0E12	0.0	1.8E3	!<estimated(x)>! *1
CH3OHC6H3CHO+R2OH= CH3C6H3OHCO+H2O	7.8E12	0.0	0.0	!<estimated(x)>! *1
CH3OHC6H3CHO+R3OOH= CH3C6H3OHCO+H2O2	3.0E12	0.0	11.0E3	!<estimated(x)>! *1
CH3OHC6H3CHO+R4CH3= CH3C6H3OHCO+CH4	2.0E-6	5.6	1.5E3	!<estimated(x)>! *1
CH3C6H3OHCO=CH3C6H4OH#+B2CO	2.0E13	0.0	30.5E3	!<estimated(y)> *1
CH3C6H4OH# + R1H = HOC6H4CH3	1.0E14	0.0	0.0	!<estimated(g)>! *1

!*****!

!*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS*!

!*****!

CH3C6H4CH2OH+O2=R3OOH+CH3C6H4CHOH	1.4E12	0.0	34.0E3	!RODA
<estimated(aaa)>! *1				
CH3C6H4CH2OH+O2=CH3C6H4CH2O+R3OOH	2.0E14	0.0	41.4E3	!<EMDEE92>! *1
CH3C6H4CH2OH+R1H=toluene+R6CH2OH	5.8E13	0.0	8.1E3	!<estimated(t)>! *1
CH3C6H4CH2OH+R1H=C6H5CH2OH+R4CH3	5.8E13	0.0	8.1E3	!<estimated(t)>! *1

CH3C6H4CH2OH+R1H=CH3C6H4CHOH+H2	8.0E13	0.0	6.4E3	!<estimated(t')>! *1
CH3C6H4CH2OH+B10=CH3C6H4CHOH+R2OH	4.2E11	0.0	-2.0E3	!<estimated(t')>! *1
CH3C6H4CH2OH+R2OH=CH3C6H4CHOH+H2O	3.5E9	1.0	-1.13E3	!<estimated(t')>! *1
CH3C6H4CH2OH+R3OOH=CH3C6H4CHOH+H2O2		2.7E11	0.0	12.0E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+R4CH3=CH3C6H4CHOH+CH4	1.1E12	0.0	9.1E3	!<estimated(t')>! *1
CH3C6H4CH2OH+C3H5Y=CH3C6H4CHOH+C3H6Y	1.1E12		0.0	13.1E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+iC4H5=CH3C6H4CHOH+C4H6Z2	1.1E12		0.0	13.1E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+nC4H5=CH3C6H4CHOH+C4H6Z2	1.112		0.0	13.1E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+C6H5#=CH3C6H4CHOH+C6H6#		5.2E13	0.0	10.0E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+C6H4CH3=CH3C6H4CHOH+toluene	5.2E13	0.0	10.0E3	!<estimated(t')>! *1
CH3C6H4CH2OH+C6H5O#=CH3C6H4CHOH+C6H5OH#	1.1E11		0.0	13.1E3
!<estimated(t')>! *1				
CH3C6H4CH2OH+benzyl=CH3C6H4CHOH+toluene	1.1E11	0.0	13.1E3	!<estimated(t')>! *1
CH3C6H4CH2OH+o-methylbenzyl=CH3C6H4CHOH+o-xylene	1.1E11	0.0	13.1E3	!<estimated(t')>! *1
!<estimated(t')>! *1				
CH3C6H4CH2OH+OC6H4CH3=CH3C6H4CHOH+HOC6H4CH3	1.1E11	0.0	13.1E3	!<estimated(t')>! *1
!<estimated(t')>! *1				
CH3C6H4CH2OH+HOC6H4CH2=CH3C6H4CHOH+HOC6H4CH3	1.1E11	0.0	13.1E3	!<estimated(t')>! *1
!<estimated(t')>! *1				
CH3C6H4CH2OH+C5H5#=CH3C6H4CHOH+C5H6#		1.1E11	0.0	13.1E3
!<estimated(t')>! *1				
CH3C6H4CHOH=CH3C6H4CHO+R1H	2.0E14	0.	23.3E3	!<asC2H5O>! *1

!*****!

!*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS*!

!*****!

!** Amorçages monomoléculaires

CH3C6H4CH2CH3 = R1H + CH3C6H4CHCH3 4.3E14 0.0 83.6E3 !<kingas>! *1

!** Amorçages bimoléculaires

CH3C6H4CH2CH3+O2=CH3C6H4CHCH3+R3OOH 1.4E12 0.0 34.0E3 !<estimated(aaa)>! *1

*1

!CH3C6H4CH2CH3+O2=C8H9#-1+R3OOH 1.2E13 0.0 49.0E3 !<exgas>!

!** Additions ipso

CH3C6H4CH2CH3+R1H=toluene+R11C2H5 5.8E13 0.0 8.1E3 !<estimated(t)>! *1

CH3C6H4CH2CH3+R1H=etC6H5+R4CH3 5.8E13 0.0 8.1E3 !<estimated(t)>! *1

!** Metatheses

CH3C6H4CH2CH3+R1H=CH3C6H4CHCH3+H2 8.0E13 0.0 6.4E3

!<estimated(t'')>! *1

CH3C6H4CH2CH3+B10=CH3C6H4CHCH3+R2OH 4.2E11 0.0 -2.0

!<estimated(t'')>! *1

CH3C6H4CH2CH3+R2OH=CH3C6H4CHCH3+H2O 3.5E9 1.0 -1.13E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+R3OOH=CH3C6H4CHCH3+H2O2 2.7E11 0.0 12.0E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+R4CH3=CH3C6H4CHCH3+CH4 1.1E12 0.0 9.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+C3H5Y=CH3C6H4CHCH3+C3H6Y 1.1E12 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+iC4H5=CH3C6H4CHCH3+C4H6Z2 1.1E12 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+nC4H5=CH3C6H4CHCH3+C4H6Z2 1.112 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+C6H5O#=#CH3C6H4CHCH3+C6H5OH# 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+benzyl=CH3C6H4CHCH3+toluene 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+o-methylbenzyl=CH3C6H4CHCH3+o-xylene 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+OC6H4CH3=CH3C6H4CHCH3+HOC6H4CH3 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+HOC6H4CH2=CH3C6H4CHCH3+HOC6H4CH3 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1
CH3C6H4CH2CH3+C5H5#=#CH3C6H4CHCH3+C5H6# 1.1E11 0.0 13.1E3
 !<estimated(t'')>! *1

!etC6H5+R1H=C8H9#-1+H2 2.8E7 2.0 7.7E3 !<exgas>!
!etC6H5+B10=C8H9#-1+R2OH 5.1E13 0.0 7.85E3 !<exgas>!
!etC6H5+R2OH=C8H9#-1+H2O 2.7E6 2.0 0.45E3 !<exgas>!
!etC6H5+R3OOH=C8H9#-1+H2O2 6.0E11 0.0 17.0E3 !<exgas>!
!etC6H5+R4CH3=C8H9#-1+CH4 0.3 4.0 8.2E3 !<exgas>!

!** Decompositions

!C8H9#-1=C2H4Z+C6H5# 7.1E14 0.0 43.5E3 !<Ebert, NIST>!
CH3C6H4CHCH3 =R1H+CH3styrene 3.1e13 0.0 50670 !<MULLER88> *1
!C8H9#-1=R1H+styrene 1.6e13 0.0 34800 !<exgas_barb>

!** Reactions of derived radicals

CH3C6H4CHCH3+O2=R3OOH+CH3styrene 7.0E11 0.0 15.0E3 !<est (exgas-sylvain)>! *1
!C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO 5.0E12 0.0 0.0 !<Kingas>!
!C8H9#-1+O2=R3OOH+styrene 1.5E12 0.0 5.0E3 !<est (exgas)>!
!C8H9#-1+R3OOH=R2OH+HCHO+benzyl 5.0E12 0.0 0.0 !<kingas>!

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

o-bibenzyl=o-C14H13#+R1H 1.0E16 0.0 83.0E3 !<Hippler>! *1
o-bibenzyl+O2=o-C14H13#+R3OOH 2.8E12 0.0 35.0E3 !<est aaaa>! *1

o-bibenzyl+R1H=o-C14H13#+H2 1.6E14 0.0 6.4E3 !<estimated(t'')>! *1

o-bibenzyl+B10=o-C14H13#+R2OH 8.4E11 0.0 -2.0 !<estimated(t'')>! *1
 o-bibenzyl+R2OH=o-C14H13#+H2O 7.0E9 1.0 -1.13E3 !<estimated(t'')>! *1
 o-bibenzyl+R3OOH=o-C14H13#+H2O2 5.4E11 0.0 12.0E3 !<estimated(t'')>! *1
 o-bibenzyl+R4CH3=o-C14H13#+CH4 2.2E12 0.0 9.1E3 !<estimated(t'')>! *1
 o-bibenzyl+C6H5O# =o-C14H13#+C6H5OH# 2.2E12 0.0 13.1e3 !<estimated(t'')>! *1
 o-bibenzyl+benzyl=o-C14H13#+toluene 2.2E12 0.0 13.1E3 !<estimated(t'')>! *1
 o-bibenzyl+o-methylbenzyl=o-C14H13#+o-xylene 2.2E12 0.0 13.1E3
 !<estimated(t'')>! *1
 o-bibenzyl+C3H5Y=o-C14H13#+C3H6Y 2.2E12 0.0 13.1E3 !<estimated(t'')>! *1
 !o-C14H13#=o-stilbene+R1H 7.1E14 0.0 30.0E3 !dd *1

!*****!
 !*REACTIONS OF BENZOCYCLOBUTANE - NAPHTHALENE AND DERIVED RADICALS*!
 !*****!

benzocyclobut + R1H = C8H9#-1 5.8E13 0.0 8.1E3 !<BAULCH94>!
 benzocyclobut = styrene 1.2e15 0.0 74.32e3 ! NIST
 benzocyclobut+o-methylbenzyl=o-xylene+benzocyclobutyl 1.6E11 0.0 15.1E3 !<estimated(a)>! *1

benzocyclobut+R1H=benzocyclobutyl+H2 1.2E14 0.0 8.4E3 !<HIPPLER90-1>
 benzocyclobut+B10=benzocyclobutyl+R2OH 6.3E11 0.0 0.0 !<HOFFMANN90>!
 benzocyclobut+R2OH=benzocyclobutyl+H2O 5.2E09 1.0 0.87E3 !<BAULCH94>!
 benzocyclobut+R3OOH=benzocyclobutyl+H2O2 4.0E11 0.0 14.0E3 !<BAULCH94>!
 benzocyclobut+R4CH3=benzocyclobutyl+CH4 1.6E12 0.0 11.1E3 !<COLKET94>!

benzocyclobutyl = styryl 7.08e+14 0.0 43.50e3 ! as phenylethyl
 styryl + R1H = styrene 1.0e14 0.0 0.0

!benzocyclobutyl + 2O2 => C6H5CHO-1 + 2B10 +R1H 6.3E12 0.0 40.0E3 !<BREZYNSKY84>!
 !C6H5CHO-1 + R1H => C6H5CHO + R5CHO 11.6E13 0.0 8.1E3

styrene=C6H6#+C2H2 1.6e11 0.0 58.44e3 !2.5E14 0.0 34E3 ! NIST
 !SQUIB : 88MUL/TRO3
 !Muller-Markgraf, W.; Troe, J.
 !Thermal decomposition of ethylbenzene, styrene, and bromophenylethane: UV absorption study in shock waves
 !J. Phys. Chem. 92, 4914 (1988)
 !Reaction : Styrene = Benzene + C2H2
 !k = 1.58e+11*exp(-58.44 kcal/RT) s**(-1) unimolecular

!benzyl + C3H3 = C10H10 1.0e10 0.0 0.0 ! MARINOV
 !2C5H5# = naphthalene + 2 R1H 4.0e13 0.0 4000.0 ! MARINOV
 !C10H10 + R2OH = C10H9 + H2O 5.0E6 2.0 0.0 ! MARINOV

!C10H10 + R1H = C10H9 + H2 2.0E5 2.5 2500.0 ! MARINOV
!C10H10 + B1O = C10H9 + R2OH 7.0E11 0.7 6000.0 ! MARINOV
!C10H10 + o-methylbenzyl = C10H9 + o-xylene 1.6E11 0.0 15.1E3 !<estimated(a)>! *1
!naphthalene + R1H = C10H9 5.0e14 0.0 5000.0 ! MARINOV

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

!*****!
!* *!
!* PRIMARY MECHANISM OF THE OXIDATION OF p-xylene *!
!* *!
!*****!

!*****!
!*REACTIONS OF p-xylene MOLECULES*!
!*****!

!**UMIMOLECULAR INITIATIONS

p-xylene = p-methylbenzyl+ R1H 0.5e16 0.0 89.0e3 !<DACOSTA00>! /2
p-xylene=C6H4CH3+R4CH3 4.0E17 0.0 97.0E3 !<COLKET94>*10! *4

!**BIMOLECULAR INITIATION

p-xylene+O2=p-methylbenzyl+R3OOH 4.2E12 0.0 38.6E3 !<estimated(aaa)> *2

!**ADDITIONS

p-xylene+R1H=toluene+R4CH3 11.6E13 0.0 8.1E3 !<BAULCH94>! *2
p-xylene+B1O=OC6H3(CH3)2+R1H 1.7E13 0.0 3.6E3 !<TAPPE89>! *1
p-xylene+R2OH=HOC6H3(CH3)2+R1H 1.3E13 0.0 10.6E3 !<BAULCH94>! *1

!**METATHESES

!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

p-xylene+R1H=p-methylbenzyl+H2 2.4E14 0.0 8.4E3 !<HIPPLER90-1>! *2
p-xylene+B1O=p-methylbenzyl+R2OH 12.6E11 0.0 0.0 !<HOFFMANN90>! *2
p-xylene+R2OH=p-methylbenzyl+H2O 10.4E9 1.0 0.87E3 !<BAULCH94>! *2
p-xylene+R3OOH=p-methylbenzyl+H2O2 8.0E11 0.0 14.0E3 !<BAULCH94>! *2
p-xylene+R4CH3=p-methylbenzyl+CH4 3.2E12 0.0 11.1E3 !<COLKET94>! *2
p-xylene+R10C2H3V=p-methylbenzyl+C2H4Z 8.0e12 0.0 8.0e3 !<COLKET94>! *2

p-xylene+C3H5Y=p-methylbenzyl+C3H6Y 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
p-xylene+C3H3=p-methylbenzyl+pC3H4 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
p-xylene+iC4H5=p-methylbenzyl+C4H6Z2 3.2E12 0.0 15.1E3 !<estimated(a)>! *2
p-xylene+nC4H5=p-methylbenzyl+C4H6Z2 3.2E12 0.0 11.1E3 !<estimated(a)>! *2
p-xylene+C5H5#=p-methylbenzyl+C5H6# 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

p-xylene+C6H5# = p-methylbenzyl+C6H6# 7.9E13 0.0 12.0E3 !<HECKMANN96>! *2
p-xylene+benzyl = p-methylbenzyl+toluene 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

p-xylene+C6H5O# = p-methylbenzyl+C6H5OH# 3.2E11 0.0 15.1E3 !<estimated(a)>! *2
p-xylene+ phenyl(CH3)2 = p-methylbenzyl+p-xylene 15.8E13 0.0 12.0E3 !<estimated(b)>! *2
p-xylene+OC6H4CH3 = p-methylbenzyl+HOC6H4CH3 3.2E11 0.0 15.1E3 !<estimated(a)>! *2
p-xylene+C6H5CH2OO = p-methylbenzyl+C6H5CH2OOH 8.0E11 0.0 14.0E3 !<estimated(c)>! *2
p-xylene+C6H5CH2O = p-methylbenzyl+C6H5CH2OH 3.2E11 0.0 11.1E3 !<estimated(a)>! *2
p-xylene+HOC6H4CH2 = p-methylbenzyl+HOC6H4CH3 3.2E11 0.0 15.1E3 !<estimated(a)>! *2

!**METATHESSES WITH ABSTRACTION OF PHENYLIC H-ATOM!

p-xylene+R1H = phenyl(CH3)2+H2 12.0E08 1.0 16.8E3 !<estimated(d)>! *1
p-xylene+B1O = phenyl(CH3)2+R2OH 4.0E13 0.0 14.7E3 !<estimated(d)>! *1
p-xylene+R2OH = phenyl(CH3)2+H2O 3.2E08 1.42 1.45E3 !<estimated(d)>! *1
p-xylene+R3OOH = phenyl(CH3)2+H2O2 11.0E12 0.0 28.9E3 !<estimated(d)>! *1
p-xylene+R4CH3 = phenyl(CH3)2+CH4 4.0E12 0.0 15.0E3 !<estimated(d)>! *1

!*****!

!**REACTIONS OF BENZYL RADICALS*

!*****!

!**DECOMPOSITION BY BETA-SCISSION

!****p-methylbenzyl => C6H7# + C2H2 6.0E13 0.0 70.0E3 !<Colket94>! *1

!**REACTIONS WITH OXYGEN

p-methylbenzyl+O2 = CH3C6H4CH2O+B1O 6.3E12 0.0 40.0E3 !<BREZYNSKY84>! *1

!**TERMINATION REACTIONS

p-methylbenzyl+B1O = C6H4CH3+HCHO 3.5E13 0.0 0.0 !<EMDEE92>! *1
p-methylbenzyl+B1O = CH3C6H4CHO+R1H 1.0E14 0.0 0.0 !<estimated(e)>! *1

p-methylbenzyl+R2OH = CH3C6H4CH2OH 2.E13 0.0 0.0 !<HIPLER91>! *1
p-methylbenzyl+R3OOH = CH3C6H4CH2OOH 5.0E12 0.0 0.0 !<HIPPLER90-2>! *1

2p-methylbenzyl = o-bibenzyl 2.5E11 0.4 0.0 !<MULLER88>! *1
!2p-methylbenzyl = bibenzyl 2.5E11 0.4 0.0 !<MULLER88>! *1

CH3C6H4CH2CH3 = p-methylbenzyl + R4CH3 3.1e15 0.0 75120 !<BAULCH94>! *1

!** ADITION

!****p-methylbenzyl + C2H2 => C10H10 + R1H 3.2e11 0.0 7000 ! MARINOV AJOUT RODA

p-methylbenzyl + O2 = p-xylylene + R3OOH 3.6E+13 0.00 13.71e3 ! NIST / *1.0
p-xylylene + R1H = p-methylbenzyl 4.1e13 0.0 1.3e3

!****p-xylylene = benzocyclobut 2.1e12 0.0 26.83e3 ! NIST
!****p-xylylene + R4CH3 => p-etC6H4 6.3e10 0.0 7500.0 ! ANALOGIE NIST
p-etC6H4 + R1H => CH3C6H4CH2CH3 1e14 0.0 0.0

!SQUIB : 88PER/RIC2

!Perrin, D.; Richard, C.; Martin, R.
!H2S-promoted thermal isomerization of Cis-2-pentene to 1-pentene and trans-2-pentene around 800 K

!Int. J. Chem. Kinet. 20, 621 (1988)
!Reaction : $\cdot\text{CH}_3 + (\text{E})\text{-CH}_2=\text{CHCH}=\text{CH}_2 = \text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3$
!k = $6.31\text{e}+10 \cdot \exp(-7.50 \text{ kcal}/\text{RT}) \text{ cm}^3/(\text{mol} \cdot \text{s})$ bimolecular

!*** a voir
p-xylylene + B10 => C6H5CHp-2 + R1H 1.0E14 0.0 0.0 !<estimated(e)>! *1 par rapport au toluene
C6H5CHp-2 + B10 => p-phtaldehyde + R1H 1.0E14 0.0 0.0 !<estimated(e)>! *1 par rapport au toluene
!****

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

!**reactions with oxygen
phenyl(CH3)2+O2=OC6H3(CH3)2+B10 2.6E13 0.0 6.1E3 !<estimated(f)>! *1

!***termination reactions!
phenyl(CH3)2+R1H=p-xylene 1.0E14 0.0 0.0 !<estimated(g)>! *1

phenyl(CH3)2+B10=OC6H3(CH3)2 1.0E14 0.0 0.0 !<estimated(f)>! *1
phenyl(CH3)2+R2OH=HOC6H3(CH3)2 1.0E13 0.0 0.0 !<estimated(f)>! *1
phenyl(CH3)2+R4CH3=trimetbenz 1.2E06 1.96 -3.7E3 !<estimation(fbis)>! *1

phenyl(CH3)2+R3OOH=OC6H3(CH3)2+R2OH 5.0E12 0.0 0.0 !<estimated(f)>! *1
phenyl(CH3)2 + R1H = p-methylbenzyl + R1H 2.0E13 0.0 0.0 !<MILLER92>! *2

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

!**Decomposition by beta-scission *****
CH3C6H4CH2O=R1H+CH3C6H4CHO 2.0E13 0.0 27.5E3 !<estimated(j)>! INHIBE *1
CH3C6H4CH2O=C6H4CH3+HCHO 2.0E13 0.0 27.5E3 !<estimated(j)>! ACCELERE *1

!***reactions with oxygen
CH3C6H4CH2O+O2=R3OOH+CH3C6H4CHO 6.0E10 0.0 1.6E3 !<estimated(k)>! *1

CH3C6H4CH2O + R1H = CH3C6H4CH2OH 2.0e13 0.0 0.0 !AJOUT RODA

benzylCH2OH + R1H = CH3C6H4CH2OH 1.0E14 0.0 0.0E3 !<estimated(g)>! *1 !
AJOUT RODA
benzylCH2OH + R2OH = HObenzylCH2OH 2.0E13 0.0 0.0 !<HIPLER91>! *1

!*****!

!*REACTIONS OF CRESOXY RADICALS*!

!*****!

!**CO elimination with rearrangement

OC6H3(CH3)2=>R1H+toluene+B2CO 3.0E11 0.0 43.8E3 !<FRANCK94>! *1

OC6H3(CH3)2=>R4CH3+C6H6#+B2CO 3.0E11 0.0 43.8E3 !<FRANCK94>! *1

!**termination reactions!

OC6H3(CH3)2+R1H=HOC6H3(CH3)2 1.0E14 0.0 0.0E3 !<estimated(g)>! *1

!*****!

!* *!

!* SECONDARY MECHANISM OF THE OXIDATION OF p-xylene *!

!* *!

!*****!

CH3C6H4CHO+p-methylbenzyl=p-xylene+CH3C6H4CO 1.3E11 0.0 11.5E3 !<estimated(p)>! *1

CH3C6H4CHO+p-methylbenzyl=p-xylene+o-C6H4CHO 1.3E11 0.0 11.5E3 !<estimated(p)>! *1

HOC6H3(CH3)2+p-methylbenzyl=OC6H3(CH3)2+p-xylene 4.9E11 0.0 9.4E3

!<estimated(s)>! *1

HOC6H3(CH3)2+p-methylbenzyl=CH3HOC6H3CH2+p-xylene 3.2E11 0.0 15.1E3

!<estimated(t)>! *2

CH3C6H4CH2OH+p-methylbenzyl=CH3C6H4CHOH+p-xylene 1.1E11 0.0 13.1E3

!<estimated(t')>! *1

CH3C6H4CH2CH3+p-methylbenzyl=CH3C6H4CHCH3+p-xylene 1.1E11 0.0 13.1E3

!<estimated(t'')>! *1

EnD