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! **                               A study of chlorobenzene pyrolysis
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! **                               N.VIN1, F.BATTIN-LECLREC1, H.LE
GALL1, N.                               ** !
! **                               SEBBAR2, H.BOCKHORN2, D.TRIMIS2,
O.HERBINET1*                               ** !
! **                               1Laboratoire Réactions et Génie des procédés, CNRS,
Université de Lorraine, BP 20451                               ** !
! **                               1 rue Grandville, 54000 Nancy, France
** !
! **                               2 Combustion Technology, Engler-Bunte-Institute,
Karlsruhe Institute of Technology (KIT)                               ** !
! **                               Engler-Bunte Ring 7, 76131 Karlsruhe,
Germany                               ** !
! **                               *Corresponding author: olivier.herbinet@univ-
lorraine.fr                               ** !
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ELEMENTS
H O C N AR HE CL
END

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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

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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
 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

! 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/1cyclohexadiene
 C6H10# !c(#1)h2/ch//ch/ch2/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
R18CH3C000 !.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
1C6H5 !ch///c/ch//ch/ch//ch(.)
1C6H7 !ex .ch//ch/ch//ch/ch//ch2
!1C6H9 !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus
(une 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

! MECHANISM OF BENZENE

! Molecules

C4H4O !ch2//ch/ch//c//o vinylketene
 !1C5H6 !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

! Radicals

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

!*Espèces ajoutées*!
!mfC5H5C2H2 !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1
!C5H4CCH2 !c(#1)h//ch/ch//ch/c(/c//ch2)/1
!C5H5CCH !c(#1)h//ch/ch//ch/ch(/c//ch)/1
C6H5COCH3 !C6H5x/CO/CH3
C8H9#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
To1OCH2C6H5 !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
indeny1
indene
cumene
CH3styre
C9H11#-1
C2H3C6H4CH2
phenanthrene
C6H5CH2CHO
!
!
!Chlorinated Compounds
HCL
CL2
CL
PHICL
R2PHICL
R3PHICL
R4PHICL

PHI12CL2
PHI13CL2
PHI14CL2
BPNL2CL
BPNL3CL
BPNL4CL
BB22CL2
BB32CL2
BB33CL2
BB42CL2
BB43CL2
BB44CL2
!C12H8 !Biphenylene
!C6JH6
!CDYC5H4
!C6H4OPEN
!C6JH7
!C6H7CL*14
!C6H7CL*13

END

THERMO

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
 TolOCH2C6H5 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
 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 0C 11H 100 0 G 0200.00 6000.00
 1
 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 0C 11H 90 0 G 0200.00 6000.00
 1
 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 0C 14H 100 0 G 0200.00 6000.00
 1
 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 0C 12H 80 0 G 0300.00 5000.00
 1
 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 0C 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 0C 10H 70 0 G 200.000 6000.000 1000.
 1
 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 0C 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
 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 110 0G 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 0C 9H 100 0G 0300.00 5000.00 1000.00
 1
 -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 0C 9H 90 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 0C 8H 80 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 70 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 0N 2C 0H 0O 0G 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 0HE 2C 0H 0O 0G 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
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	20	0
1			G	0300.00
				5000.00
				1000.00
-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	40	0
1			G	0300.00
				5000.00
				1000.00
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	60	0
1			G	0300.00
				5000.00
				1000.00
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	20	1
1			G	0300.00
				5000.00
				1000.00
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	40	1
1			G	0300.00
				5000.00
				1000.00
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	60	1
1			G	0300.00
				5000.00
				1000.00
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	60	2
1			G	0300.00
				5000.00
				1000.00
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 0C 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
 14 2
 -1.18838341E+04 -1.49881933E+01 4.69868861E+00 4.99965957E-03 4.38587397E-05
 05 3
 -6.12883900E-08 2.48508985E-11 -1.00875286E+04 7.29812046E+00 -
 8.18629119E+03 4

CH2CHCO MF-BURCAT 0C 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
 14 2
 8.15590313E+03 -1.21011994E+01 3.13639619E+00 1.99890906E-02 -7.99294937E-06
 06 3
 -4.77227085E-09 3.89527783E-12 9.50725768E+03 1.18910245E+01
 1.12526174E+04 4

C3H2 0H 2C 3 0 0G 0150.00 4000.00 1000.00
 1
 7.67098100E+00 2.74874900E-03 -4.37094300E-07 -6.45559900E-11 1.66388700E-14
 14 2
 6.25972200E+04 -1.23689000E+01 3.16671400E+00 2.48257200E-02 -4.59163700E-05
 05 3
 4.26801900E-08 -1.48215200E-11 6.35042100E+04 8.86944600E+00
 4

pC3H4 0C 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
 13 2
 0.19653348E+05 -0.83392105E+01 0.20619018E+01 0.20599686E-01 -0.10556581E-04
 04 3
 0.13453347E-08 0.47999533E-12 0.20849322E+05 0.12362522E+02
 4

aC3H4 0C 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
 13 2
 0.20362814E+05 -0.97686501E+01 0.11219990E+01 0.24131576E-01 -0.14620023E-04
 04 3
 0.33471641E-08 0.90883478E-13 0.21810221E+05 0.16326361E+02
 4

C3H6Y 0C 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 0C 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 0C 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 0C 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 0C 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 0C 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 0C 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 60 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 60 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 60 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 80 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 60 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 0C 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 0C 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 5O 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 5O 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 5O 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
 1C6H4 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
 1C6H6 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
 1C6H8 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
 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

```


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
 1C6H5 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
 1C6H7 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
 1C6H9 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 4O 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 3O 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 9O 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 8O 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 9O 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 8O 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 7O 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
 1C5H6 0C 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 0C 5H 4O 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 0C 5H 6O 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# 0C 6H 6O 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 0C 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 0C 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 0C 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 60 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 0C 8H 100 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 0C 8H 80 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 0C 9H 80 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 0C 10H 100 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 g 8/00C 12.H 10. 0. 0.G 200.000 6000.000 1000.
1
2.28963620E+01 3.68453189E-02-1.35016357E-05 2.20802787E-09-1.33358137E-
13 2
1.07395923E+04-1.00509573E+02 1.94600056E-01 5.35259888E-02 8.55000841E-
05 3
-1.63903525E-07 7.29975666E-11 1.90021492E+04 2.72148992E+01
2.19050792E+04 4
C5H5# MF-BURCAT 0C 5H 5 G 0300.00 5000.00 1000.00
1
1.02615305E+01 1.55578917E-02-5.54166182E-06 8.89865066E-10-5.30836089E-
14 2
2.80714257E+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
1C5H5 0C 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
 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 0C 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 0C 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 0C 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 0C 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 0C 7H 7O 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 0C 7H 7O 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 0C 7H 5O 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 0C 7H 7O 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 0C 7H 7O 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 0C 7H 7O 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 0C 7H 7O 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# 0C 8H 9O 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 0C 8H 9O 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 0C 8H 7O 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# 0C 14H 13O 0G 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 BURCAT 0C 7H 8O 1 G 0300.00 5000.00 1000.00
 1
 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 0C 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 0C 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 0C 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 0C 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 0C 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 80 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 80 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 70 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 70 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 70 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 70 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 70 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 70 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 70 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 70 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 70 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 90 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 90 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 100 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 90 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 90 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 90 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 90 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 80 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 70 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 70 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
 !Chlorinated compounds
 HCL ATcT3CCL 1.H 1. 0. 0.G 200.000 6000.000 1000.
 1

2.75038607E+00 1.46525702E-03-4.85796370E-07 7.90400572E-11-4.88097333E-
 15 2
 -1.18941369E+04 6.56298585E+00 3.46434022E+00 4.74166973E-04-2.00403781E-
 06 3
 3.32826880E-09-1.45873238E-12-1.21280024E+04 2.66176266E+00-
 1.10858645E+04 4
 CL2 REF ELEMENT ATcT3CCL 2. 0. 0. 0.G 200.000 6000.000 1000.
 1
 4.72497332E+00-4.52025622E-04 2.48339908E-07-1.98734964E-11-1.38247235E-
 15 2
 -1.50144014E+03-2.18753211E-01 2.74354106E+00 7.78656796E-03-1.44041508E-
 05 3
 1.24869963E-08-4.11292285E-12-1.05955046E+03 9.41507624E+00
 0.00000000E+00 4
 CL ATcT3CCL 1. 0. 0. 0.G 200.000 6000.000 1000.
 1
 2.96123231E+00-4.06760214E-04 1.45948930E-07-2.36008477E-11 1.41691234E-
 15 2
 1.36901066E+04 3.02880221E+00 2.23418328E+00 1.73391135E-03-1.15488156E-
 06 3
 -1.12443736E-09 9.89461388E-13 1.38580303E+04 6.68075708E+00
 1.45892781E+04 4
 PHICL C 6H 5CL 1 0G 300.000 5000.000
 1400.000 01!
 1.67464346E+01 1.40444495E-02-4.55123150E-06 6.84556856E-10-3.90121847E-
 14 2
 -2.01380675E+03-6.62503036E+01-3.87969886E+00 6.89925268E-02-6.09983756E-
 05 3
 2.70515626E-08-4.72867550E-12 4.36554009E+03 4.19479242E+01
 4
 R2PHICL C 6H 4CL 1 0G 300.000 5000.000
 1278.000 01
 1.64452814E+01 1.19352714E-02-3.89316656E-06 5.88324994E-10-3.36384759E-
 14 2
 3.02608068E+04-6.20679730E+01-2.82971324E+00 6.39589926E-02-5.80570392E-
 05 3
 2.62102161E-08-4.64205612E-12 3.61542124E+04 3.88022935E+01
 4
 R3PHICL C 6H 4CL 1 0G 300.000 5000.000
 1294.000 01
 1.65036978E+01 1.18799882E-02-3.87664167E-06 5.85907071E-10-3.35002922E-
 14 2
 2.93585052E+04-6.24563467E+01-2.90725131E+00 6.45347728E-02-5.89855456E-
 05 3
 2.67848553E-08-4.76657491E-12 3.52680751E+04 3.90333530E+01
 4
 R4PHICL C 6H 4CL 1 0G 300.000 5000.000
 1287.000 01
 1.64973432E+01 1.18720158E-02-3.86506805E-06 5.83371893E-10-3.33303968E-
 14 2
 2.96624838E+04-6.24338225E+01-2.88463041E+00 6.43778837E-02-5.87270723E-
 05 3
 2.66185180E-08-4.72864455E-12 3.55682939E+04 3.89260529E+01
 4
 PHI12CL2 C 6H 4CL 2 0G 300.000 5000.000
 1305.000 01
 1.90847407E+01 1.21551815E-02-3.92974665E-06 5.91724844E-10-3.37974048E-
 14 2

-4.88961026E+03-7.47292311E+01-1.78024741E+00 6.88137130E-02-6.32765178E-
 05 3
 2.88226616E-08-5.13658842E-12 1.45434092E+03 3.43382054E+01
 4
 PHI13CL2 C 6H 4CL 2 OG 300.000 5000.000
 1311.000 01
 1.91087550E+01 1.21249493E-02-3.92043871E-06 5.90270665E-10-3.37085965E-
 14 2
 -5.48016357E+03-7.46622167E+01-1.71158247E+00 6.88146605E-02-6.34718787E-
 05 3
 2.89982940E-08-5.18157324E-12 8.36333695E+02 3.41199976E+01
 4
 PHI14CL2 C 6H 4CL 2 OG 300.000 5000.000
 1309.000 01
 1.90838772E+01 1.21523181E-02-3.92949675E-06 5.91629625E-10-3.37855760E-
 14 2
 -5.48766909E+03-7.45194506E+01-1.68993810E+00 6.86699668E-02-6.32550376E-
 05 3
 2.88731605E-08-5.15594813E-12 8.19532889E+02 3.40362669E+01
 4
 BPNL4CL C 12H 9CL 1 OG 300.000 5000.000
 1400.000 01
 0.46692513E+02 0.25427334E-02-0.14477476E-06-0.33360992E-11 0.80836738E-
 15 2
 -0.25601094E+04-0.23000021E+03-0.63855391E+01 0.11364487E+00-0.72034942E-
 04 3
 0.12858743E-07 0.99982143E-12 0.15514940E+05 0.56955818E+02
 4
 BPNL3CL C 12H 9CL 1 OG 300.000 5000.000
 1400.000 01
 0.46692513E+02 0.25427334E-02-0.14477476E-06-0.33360992E-11 0.80836738E-
 15 2
 -0.25601094E+04-0.22930713E+03-0.63855391E+01 0.11364487E+00-0.72034942E-
 04 3
 0.12858743E-07 0.99982143E-12 0.15514940E+05 0.57648903E+02
 4
 BPNL2CL C 12H 9CL 1 OG 300.000 5000.000
 1400.000 01
 0.46692513E+02 0.25427334E-02-0.14477476E-06-0.33360992E-11 0.80836738E-
 15 2
 -0.22581758E+04-0.22930713E+03-0.63855391E+01 0.11364487E+00-0.72034942E-
 04 3
 0.12858743E-07 0.99982143E-12 0.15816874E+05 0.57648903E+02
 4
 BB44CL2 C 12H 8CL 2 OG 300.000 5000.000
 1510.000 01
 6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
 14 2
 -1.64978770E+04-3.41890178E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
 05 3
 -1.17383304E-09 5.26356430E-12 1.15213737E+04 5.36185090E+01
 4
 BB43CL2 C 12H 8CL 2 OG 300.000 5000.000
 1510.000 01
 6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
 14 2
 -1.64978770E+04-3.40158924E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
 05 3

-1.17383304E-09 5.26356430E-12 1.15213737E+04 5.53497621E+01
4
BB42CL2 C 12H 8CL 2 OG 300.000 5000.000
1510.000 01
6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
14 2
-1.64978770E+04-3.40158924E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
05 3
-1.17383304E-09 5.26356430E-12 1.15213737E+04 5.53497621E+01
4
BB33CL2 C 12H 8CL 2 OG 300.000 5000.000
1510.000 01
6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
14 2
-1.64978770E+04-3.40158924E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
05 3
-1.17383304E-09 5.26356430E-12 1.15213737E+04 5.53497621E+01
4
BB32CL2 C 12H 8CL 2 OG 300.000 5000.000
1510.000 01
6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
14 2
-1.64978770E+04-3.39811667E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
05 3
-1.17383304E-09 5.26356430E-12 1.15213737E+04 5.56970193E+01
4
BB22CL2 C 12H 8CL 2 OG 300.000 5000.000
1510.000 01
6.59373007E+01-1.48068303E-02 2.21727696E-07 5.57756369E-10-5.61820855E-
14 2
-1.64978770E+04-3.40158924E+02-5.32883183E+00 1.12924809E-01-6.26280488E-
05 3
-1.17383304E-09 5.26356430E-12 1.15213737E+04 5.53497621E+01
4
C12H8 biphenylen T 8/14C 12.H 8. 0. 0.G 200.000 6000.000 1000.
1
2.14943346E+01 3.31238854E-02-1.20651081E-05 1.96677465E-09-1.18566034E-
13 2
3.97273863E+04-9.46644256E+01-9.26510662E-01 5.29144662E-02 7.56324038E-
05 3
-1.51364316E-07 6.81452776E-11 4.77004412E+04 3.06183525E+01
5.01773406E+04 4
END

REACTIONS

!*****
***!
!especes excitees!
R1H+B1O+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+B1O=R2OH+B1O	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+B1O=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>!				
B1O+R4CH3=R7CH3O	8.0E15	-2.12	0.6E3	
! (61,-61) <DEAn87nIS>!				
B1O+CH4=R4CH3+R2OH	7.2E8	1.56	8.4E3	
! (62,-62) <BAULCH94>!				
B1O+R9C2H=B4CH+B2CO	1.0E13	0.	0.	
! (63,-63) <DAGAUT91>!				
B1O+C2H2=B5CH2+B2CO	2.17E06	2.1	1.6E3	
! (64,-64) <BAULCH LEEDS>!				
B1O+C2H2=R12CHCOZ+R1H	5.06E06	2.1	1.6E3	
! (65,-65) <BAULCH LEEDS>!				
R2OH+R9C2H=C2H2+B1O	1.8E13	0.	0.	! (89,-
89) <TSANG86>! modif MF				
B1O+R10C2H3V=R4CH3+B2CO	3.0E13	0.	0.	
! (66,-66) <DAGAUT91>!				
B1O+R10C2H3V=CH2COZ+R1H	9.6E13	0.	0.	
! (67,-67) <TSAnG86>!				
B1O+C2H4Z=R4CH3+R5CHO	8.1E6	1.88	0.2E3	
! (68,-68) <BAULCH94>!				
B1O+C2H4Z=HCHO+B5CH2	4.00E5	1.88	0.2E3	
! (69,-69) <BAULCH94>!				
B1O+C2H4Z=CH2COZ+H2	6.6E5	1.88	0.2E3	
! (70,-70) <BAULCH94>!				
B1O+C2H4Z=R13CH2CHO+R1H	4.7E6	1.88	0.2E3	
! (71,-71) <BAULCH94>!				
B1O+C2H4Z=R2OH+R10C2H3V	1.5E7	1.91	3.7E3	
! (72,-72) <MAHMUD87nIST>!				
B1O+R11C2H5=HCHO+R4CH3	1.1E13	0.	0.	
! (73,-73) <BAULCH94>!				
B1O+R11C2H5=CH3CHO+R1H	5.5e13	0.	0.	
! (74,-74) <BAULCH94>!				
B1O+R11C2H5=C2H4Z+R2OH	3.0E13	0.	0.	
! (75,-75) <DAGAUT91>!				
B1O+C2H6=R11C2H5+R2OH	1.0E9	1.5	5.8E3	
! (76,-76) <BAULCH94>!				

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

R1H+B1O+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/				

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!      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+B1O     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+B1O        1.5E9       1.14      0.1E3
      ! (102,-102)<BAULCH94>!

!***** REACTIONS DE H2O *****!
H2O+B4CH=R6CH2OH         5.7E12      0.        -0.8E3
      ! (103,-103)<BAULCH94>!

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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+B1O+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=B1O+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+B1O=R1H+CO2	3.0E13	0.	0.
! (121,-121)<BAULCH94>!			
R5CHO+B1O=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+B1O=R5CHO+R2OH 4.1E11 0.57 2.7E3
 ! (130,-130)<BAULCH94>!
 HCHO+R2OH=R5CHO+H2O 7.82E07 1.63 -1.06E3 !MF
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!***** REACTIONS DE R7CH3O *****!

R7CH3O+M=HCHO+R1H+M 1.55E14 0.00 13.5E3
 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+B10=HCHO+R2OH	4.2E13	0.	0.	
!(165,-165)<TSAnG87>!				
R6CH2OH+R2OH=H2O+HCHO	2.4E13	0.	0.	
!(166,-166)<TSAnG87>!				
!attention (167) metatheses dans les reactions de CH3OH!				
!R6CH2OH+H2O=CH3OH+R2OH	1.6E14	0.	26.3E3	
!(167,-167)<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+B1O=R6CH2OH+R2OH	3.4E13	0.	5.5E3	! (182,-
182)<GROTHER81nIST>!				
CH3OH+B1O=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 R12CHCOD *****!

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+B1O=>B2CO+B2CO+R1H	9.6E13	0.	0.	
! (190)<BAULCH94>!				
R12CHCOZ+R2OH=>R5CHO+B2CO+R1H	1.0E13	0.	0.	
! (191)<DAGAUT91>!				

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

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+B1O=B5CH2+CO2 1.8E12 0. 1.3E3
! (197,-197)<DAGAUT91>!
CH2COZ+B1O=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+B1O=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+B1O=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+B1O=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 *****!

B1O+B1O+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+B1O 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/		!k0
BAULCH94!						
	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)=R8CH3OO(+M)			7.8E8	1.2	0.	!(257,-
257)<BAULCH94>!						
	LOW	/5.6E25	-3.3	0./		
	TROE	/0.36	1.0	1.0E8/		
O2+R4CH3=R7CH3O+B1O			1.3E14	0.	31.3E3	!(258,-
258)<BAULCH94>!						
!O2+R4CH3=R7CH3O+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+R3OOH			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+R3OOH			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+R3OOH			1.2E11	0.	0.	!(265,-
265)<TSAnG86>!						

!O2+R10C2H3V=C2H2+R3OOH 265)<WAnG97>! !at 760 Torr	1.6E14	-0.83	2.5E3	!(265,-
!O2+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	8.6E21	-2.97	3.3E3	!(266a,-
!O2+R10C2H3V=B1O+R13CH2CHO 266b)<WAnG97>! !at 20-90 Torr	1.2E13	-0.12	1.7E3	!(266b,-
!O2+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	1.6E21	-2.78	2.5E3	!(266a,-
!O2+R10C2H3V=B1O+R13CH2CHO 266b)<WAnG97>!	2.5E12	0.057	0.9E3	!(266b,-
O2+R10C2H3V=C2H2+R3OOH 265)<MEBEL nIST>!	1.34E6	1.61	-0.4E3	!(265,-
O2+R10C2H3V=HCHO+R5CHO 266a)<MEBEL nIST>!	4.5E16	-1.39	1.0E3	!(266a,-
O2+R10C2H3V=B1O+R13CH2CHO 266b)<MEBEL nIST>!	3.3E11	-0.29	10.	!(266b,-
O2+C2H4Z=R10C2H3V+R3OOH 267)<TSAnG86>!	4.2E13	0.	57.4E3	!(267,-
O2+R11C2H5=R17C2H5OO 268)<WAGnER90>!	2.2E10	0.77	-0.6E3	!(268,-
O2+R11C2H5=C2H4Z+R3OOH 269)<TSAnG86>!	8.4E11	0.	3.9E3	!(269,-
O2+R11C2H5=R15C2H5O+B1O 270)<BOZZELLI90nIST>!	1.2E13	-0.2	27.9E3	!(270,-
O2+R11C2H5=CH3CHO+R2OH 271)<TSAnG86>!	6.0E10	0.	6.9E3	!(271,-
O2+C2H6=R11C2H5+R3OOH 272)<BAULCH94>!	6.0E13	0.	51.7E3	!(272,-
O2+R2OH=R3OOH+B1O 273)<TSAnG86>!	2.2E13	0.	52.5E3	!(273,-
O2+B2CO=CO2+B1O 274)<TSAnG86>!	2.5E12	0.	47.7E3	!(274,-
!O2+R5CHO=B2CO+R3OOH 275)<TSAnG86>!	5.1E13	0.	1.7E3	!(275,-
O2+R5CHO=B2CO+R3OOH 275)<TIMOnEn88>!	7.6E12	0.	0.41E3	!(275,-
O2+HCHO=R5CHO+R3OOH 276)<TSAnG86>!	2.0E13	0.	38.8E3	!(276,-
O2+R7CH3O=HCHO+R3OOH 277)<BAULCH94>!	2.2E10	0.	1.7E3	!(277,-
O2+R6CH2OH=HCHO+R3OOH 278)<TSAnG87>!	1.2E12	0.	0.	!(278,-
O2+CH3OH=R6CH2OH+R3OOH 279)<TSAnG87>!	2.0E13	0.	44.9E3	!(279,-
O2+R12CHCOZ=>B2CO+B2CO+R2OH <DAGAUT91>!	1.5E12	0.	2.5E3	!(280)
!O2+CH2COZ=HCHO+CO2 281)<DAGAUT91>!bizarre	1.0E8	0.	0.	!(281,-
O2+R14CH3CO=R18CH3COOO 282)<COX90>!	2.4E12	0.	0.	!(282,-
O2+R13CH2CHO=>HCHO+R2OH+B2CO <COX90>!	5.9E9	0.	-1.4E3	!(283)
O2+R13CH2CHO=CH2COZ+R3OOH 284)<COX90>!	1.0E10	0.	-1.4E3	!(284,-

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 111(2007)4031 - 4042
 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+B1O=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 326) <TSAnG86>!	1.8E13	0.	0. ! (326,-
R8CH3OO+R4CH3=R7CH3O+R7CH3O 327) <CAVAnAGH90>!	5.0E12	0.	-1.4E3 ! (327,-
R8CH3OO+CH4=CH3OOH+R4CH3 328) <TSAnG86>!	1.8E11	0.	18.5E3 ! (328,-
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ 329) <TSAnG86>!	2.4E13	0.	0. ! (329,-
!R8CH3OO+C2H2=CH3OOH+R9C2H 330) <RAnZI94>! MF car i<<0	5.6E11	0.	24.5E3 ! (330,-
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 331) <TSAnG86*>!	2.4E13	0.	0. ! (331,-
!* assuming that C2H3O decompose rapidly to R13CH2CHO!			
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3 332) <nIKISHA81/MOSHKInA80nIST>!	1.1E15	0.	20.0E3 ! (332,-
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V 333) <RAnZI94>!	3.9E12	0.	24.5E3 ! (333,-
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O 334) <TSAnG86>!	2.4E13	0.	0. ! (334,-
R8CH3OO+C2H6=CH3OOH+R11C2H5 335) <TSAnG86>!	2.9E11	0.	14.9E3 ! (335,-
R8CH3OO+B1O=R7CH3O+O2 336) <TSAnG86>!	3.6E13	0.	0. ! (336,-
R8CH3OO+R2OH=CH3OH+O2 337) <TSAnG86>!	6.0E13	0.	0. ! (337,-
R8CH3OO+R2OH=R7CH3O+R3OOH 338) <RAnZI94>!	3.0E12	0.	0. ! (338,-
R8CH3OO+B2CO=R7CH3O+CO2 339) <RAnZI94>!	1.0E14	0.	24.0E3 ! (339,-
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2 <TSAnG86>!	3.0E13	0.	0. ! (340)
R8CH3OO+HCHO=CH3OOH+R5CHO 341) <CAVAnAGH90>!	1.0E12	0.	12.1E3 ! (341,-
R8CH3OO+R7CH3O=HCHO+CH3OOH 342) <TSAnG86>!	3.0E11	0.	0. ! (342,-
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO ! (343) <TSAnG87>!	1.2E13	0.	0.
R8CH3OO+CH3OH=CH3OOH+R6CH2OH 344) <TSAnG87>!	1.8E12	0.	13.7E3 ! (344,-
R8CH3OO+CH3OH=CH3OOH+R7CH3O 345) <RAnZI94>!	2.8E11	0.	18.8E3 ! (345,-
R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ 346) <RAnZI94>!	1.7E12	0.	27.0E3 ! (346,-
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O 347) <TSAnG86>!	2.4E13	0.	0. ! (347,-
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO 348) <CAVAnAGH90>!	1.0E12	0.	12.1E3 ! (348,-
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO 349) <RAnZI94>!	1.7E12	0.	19.2E3 ! (349,-
R8CH3OO+C2H4O#3=CH3OOH+R13CH2CHO 350) <RAnZI94>!	2.2E12	0.	16.0E3 ! (350,-
R8CH3OO+R3OOH=CH3OOH+O2 351) <BAULCH94>!	2.5E11	0.	-1.6E3 ! (351,-
R8CH3OO+R3OOH=>O2+HCHO+H2O ! (352) <RAnZI94>!	5.0E10	0.	0.
R8CH3OO+H2O2=CH3OOH+R3OOH 353) <TSAnG86>!	2.4E12	0.	9.9E3 ! (353,-

R8CH3OO+R8CH3OO=CH3OH+HCHO+O2 2.5E10 0. -0.8E3 !(354,-
354)<BAULCH94>!
R8CH3OO+R8CH3OO=R7CH3O+R7CH3O+O2 2.5E10 0. -0.8E3 !(355,-
355)<BAULCH94>!

!***** REACTIOOnS DE CH3OOH *****!

CH3OOH=R7CH3O+R2OH 6.0E14 0. 42.3E3 !(356,-
356)<BAULCH94>!
CH3OOH+B1O=R8CH3OO+R2OH 2.0E13 0. 4.8E3 !(357,-
357)<BAULCH94average>!
CH3OOH+R2OH=H2O+R8CH3OO 1.8E12 0. -0.37E3 !(358,-
358)<BAULCH94average>!
CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO 1.5E11 0. 6.5E3
!(359)<RAnZI94>!

!***** REACTIOOnS DE R17C2H5OO *****!

R17C2H5OO=R16C2H4OOH 4.2E12 0. 36.9E3 !(360,-
360)<HUGHES93>!
R17C2H5OO+H2=C2H5OOH+R1H 7.9E12 0. 21.0E3 !(361,-
361)<RAnZI94>!
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O 2.0E12 0. -1.2E3 !(362,-
362)<RAnZI94>!
R17C2H5OO+CH4=C2H5OOH+R4CH3 3.9E12 0. 24.0E3 !(363,-
363)<RAnZI94>!
R17C2H5OO+C2H2=C2H5OOH+R9C2H 5.6E11 0. 24.4E3 !(364,-
364)<RAnZI94>!
R17C2H5OO+C2H4Z=C2H5OOH+R10C2H3V 3.9E12 0. 24.4E3 !(365,-
365)<RAnZI94>!
R17C2H5OO+C2H4Z=R15C2H5O+C2H4O#3 2.3E16 0. 21.9E3 !(366,-
366)<MOSHKIInA80nIST>!
R17C2H5OO+C2H6=C2H5OOH+R11C2H5 5.1E12 0. 19.5E3 !(367,-
367)<RAnZI94>!
R17C2H5OO+H2O=C2H5OOH+R2OH 5.6E12 0. 30.6E3 !(368,-
368)<RAnZI94>!
R17C2H5OO+B2CO=CO2+R15C2H5O 1.0E14 0. 24.0E3 !(369,-
369)<RAnZI94>!
R17C2H5OO+HCHO=C2H5OOH+R5CHO 4.5E12 0. 14.4E3 !(370,-
370)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R7CH3O 2.8E11 0. 18.4E3 !(371,-
371)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R6CH2OH 2.8E12 0. 19.5E3 !(372,-
372)<RAnZI94>!
R17C2H5OO+CH2COZ=C2H5OOH+R12CHCOZ 1.7E12 0. 24.4E3 !(373,-
373)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R14CH3CO 3.9E12 0. 14.4E3 !(374,-
374)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R13CH2CHO 1.7E12 0. 19.5E3 !(375,-
375)<RAnZI94>!
R17C2H5OO+C2H4O#3=C2H5OOH+R13CH2CHO 2.2E12 0. 16.3E3 !(376,-
376)<RAnZI94>!
R17C2H5OO+R3OOH=O2+C2H5OOH 3.9E11 0. -1.3E3 !(377,-
377)<BAULCH89>!
!Rate constant measured between 240 and 380K!
R17C2H5OO+H2O2=C2H5OOH+R3OOH 4.5E11 0. 10.8E3 !(378,-
378)<RAnZI94>!
R17C2H5OO+R8CH3OO=>R15C2H5O+R7CH3O+O2 2.0E11 0. 0.
!(379)<RAnZI94>!

R17C2H5OO+CH3OOH=C2H5OOH+R8CH3OO 1.1E12 0. 16.3E3 !(380,-
 380)<RAnZI94>!
 R17C2H5OO+R17C2H5OO=2R15C2H5O+O2 4.1E10 0. 0.2E3 !(381,-
 381)<LIGHTFOOT92>!
 R17C2H5OO+R17C2H5OO=C2H5OH+CH3CHO+O2 1.8E10 0. 0.2E3 !(382,-
 382)<LIGHTFOOT92>!

!***** REACTIONS DE R16C2H4OOH *****!

R16C2H4OOH=C2H4O#3+R2OH 1.5E11 0. 20.0E3 !(383,-
 383)<RAnZI94>!
 R16C2H4OOH=R6CH2OH+HCHO 2.5E13 0. 27.5E3 !(384,-
 384)<RAnZI94>!
 R16C2H4OOH=C2H4Z+R3OOH 2.0E13 0. 23.5E3 !(385,-
 385)<RAnZI94>!

!***** REACTIONS DE C2H5OOH *****!

C2H5OOH=R15C2H5O+R2OH 4.0E15 0. 42.9E3 !(386,-
 386)<BAULCH94>!
 C2H5OOH+R1H=>CH3CHO+R2OH+H2 3.2E13 0. 7.7E3
 !(387)<RAnZI94>!
 C2H5OOH+R4CH3=>CH3CHO+R2OH+CH4 5.7E11 0. 8.7E3
 !(388)<RAnZI94>!
 C2H5OOH+R9C2H=>CH3CHO+R2OH+C2H2 6.0E11 0. 9.2E3
 !(389)<RAnZI94>!
 C2H5OOH+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12 0. 8.7E3
 !(390)<RAnZI94>!
 C2H5OOH+R11C2H5=>CH3CHO+R2OH+C2H6 3.4E11 0. 11.4E3
 !(391)<RAnZI94>!
 C2H5OOH+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+B1O=CH3CHCO+2R1H	5.0E7	1.76	-1.22E3
!<TSAng91>!			
!CH3CHCO+R2OH=CH2CHCO+H2O	4.0E6	2.0	0.0
!<MARInOV>!			
!CH3CHCO+B1O=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+B1O=R4CH3+R5CHO+B2CO	3.0E7	2.0	0.0
!<MARInOV>!			
!tC3H5+O2=CH3CHCO+R1H+B1O	1.6E15	-0.78	3.1E3
!<MARInOV>!			
!tC3H5+B1O=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+B1O=CH2CHCO+R2OH	7.2E12	0.0	2.0E3
!<MARInOV>!			
C2H3CHO+B1O=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+B1O=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+B1O=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+B1O=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 !<MILLER87/BAULCH94>!	1.8E14	0.0	0.0
C3H3+R1H=C3H2+H2 !<MILLER92/BRAUn89>!	2.0E13	0.0	0.0
C3H3+B1O=R9C2H+HCHO !<MILLER92/SLAGUE91>!	1.4E14	0.0	0.0
C3H3+R2OH=C3H2+H2O !<MILLER92>!	2.0E13	0.0	0.0
C3H3+R2OH=R10C2H3V+R5CHO !<WAnG97>!	4.0E13	0.0	0.0
C2H2+R12CHCOZ=C3H3+B2CO !<MILLER92>!	1.0E11	0.0	3.0E3
C3H3+O2=CH2COZ+R5CHO !<MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3
C3H2+R1H=C3H3 !<est>!	1.0E14	0.0	0.0
C3H3+R3OOH=>R2OH+R9C2H+HCHO !<Heyberger>!	1.0E15	-0.8	0.0
C3H3+C3H3=C6H6# !<STEIn90>shocktube!	1.0E12	0.0	0.0
C3H3+C3H3=C6H5#+R1H !<STEIn90>flame!	1.0E12	0.0	0.0

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

!pC3H4=>aC3H4 !<HIDAKA89>!	2.1E12	0.0	60.0E3
pC3H4+M=C3H3+R1H+M !<HIDAKA89>!	4.7E18	0.0	80.0E3
C2H2+B5CH2=pC3H4 !<TSAnG86>!	3.5E12	0.0	0.0
pC3H4=R9C2H+R4CH3 !<KInGAS1500>!	4.2E15	0.0	125.0E3
pC3H4+O2=C3H3+R3OOH !<est Ingham>!	2.1E12	0.0	40.8E3
pC3H4+R1H=C2H2+R4CH3 !<hidaka89> !	1.3E5	2.5	1.00E3
pC3H4+R1H (+M) =tC3H5 (+M) !<WAGnER72>!	8.5E12	0.0	1.7E3
LOW /5.6E25	-7.27	6.58E3/	
!<Marinov97!			
pC3H4+R1H (+M) =sC3H5 (+M) ! <WAGnER72>!	5.8E12	0.0	3.1E3
LOW /3.8E25	-7.27	7.98E3/	
!<estimated>!			
pC3H4+R4CH3=C3H3+CH4 !<asTSAnG91>!	2.2E0	3.5	5.7E3
pC3H4+R1H=C3H3+H2 !<asTSAnG91>	1.7E5	2.5	2.5E3
pC3H4+R9C2H=C3H3+C2H2 !<asTSAnG91>!	3.6E12	0.0	0.0

pC3H4+R10C2H3V=C3H3+C2H4Z !<asTSAnG91>!	2.2E0	3.5	4.7E3
pC3H4+R11C2H5=C3H3+C2H6 !<asTSAnG91>!	2.2E0	3.5	6.6E3
pC3H4+B10=R12CHCOZ+R4CH3 !<WARnATZ84>!	1.5E13	0.0	2.1E3
pC3H4+B10=R2OH+C3H3 !<<ADUSEI, G.Y, 1996>!	3.4E4	2.16	4.8E3
pC3H4+R2OH=CH2COZ+R4CH3 !<BOODAGHIANs87>!	4.3E11	0.0	-0.8E3
pC3H4+R2OH=R1H+C2H3CHO !<asBOODAGHIANs87>!	4.3E11	0.0	-0.8E3
pC3H4+R2OH=C3H3+H2O !<asTSAnG91>!	3.1E6	2.0	-0.3E3
pC3H4+R3OOH=C2H4Z+B2CO+R2OH !as296<TSAnG86>!	6.0E9	0.0	8.0E3
pC3H4+R3OOH=C3H3+H2O2 !<asTSAnG91>!	9.6E3	2.6	13.9E3
pC3H4+R7CH3O=CH3OH+C3H3 !<Heyberger>!	2.0E12	0.0	4.0E3

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

aC3H4=pC3H4 !<HIDAKA89>!	2.5E12	0.0	59.0E3
aC3H4+M=C3H3+R1H+M !<HIDAKA89>!	2.0E18	0.0	80.0E3
aC3H4+O2=C3H3+R3OOH !<Estimation Ingham>!	2.8E13	0.0	39.0E3
aC3H4+R1H(+M)=C3H5Y(+M) 2.7E3 !<WAGnER72>!		4.0E12	0.0
LOW /5.6E33 -5.0 4.44E3/ !<Marinov97> !			
aC3H4+R1H(+M)=tC3H5(+M) !<WAGnER72>!	8.5E12	0.0	2.0E3
LOW /1.1E34 -5.0 4.44E3/ !<Marinov97!			
C2H4Z+B4CH=aC3H4+R1H !<BAULCH94base>!	1.3E14	0.0	-0.3E3
R10C2H3V+B5CH2=aC3H4+R1H !<MILLER92>!	3.0E13	0.0	0.0
iC4H3+B5CH2=aC3H4+R9C2H !<MILLER92>!	2.0E13	0.0	0.0
aC3H4+B10=R1H+B2CO+R10C2H3V !<Aleksandrev nist>!	6.6E12	0.0	3.0E3
aC3H4+R2OH=CH2COZ+R4CH3 !<LIU88>!	2.0E12	0.0	-0.2E3
aC3H4+R2OH=HCHO+R10C2H3V !<LIU88>!	2.0E12	0.0	-0.2E3
aC3H4+R1H=C3H3+H2 !<est.butatiene>!	1.3E6	2.53	9.2E3
aC3H4+B10=C3H3+R2OH !<fromAleksandrev nist>!	6.2E12	0.0	1.9E3
!d'après leur vitesse de réaction total et d'addition !			
aC3H4+R2OH=C3H3+H2O !<est.butadiene>!	6.2E6	2.0	0.4E3

aC3H4+R4CH3=C3H3+CH4 !<WU87>!	2.0E12	0.0	7.7E3
aC3H4+R9C2H=C3H3+C2H2 !<WU87>!	1.0E13	0.0	0.0
aC3H4+C3H5Y=C3H3+C3H6Y !<DAGAUT92>	2.0E12	0.0	7.7E3
aC3H4+R7CH3O=CH3OH+C3H3 9.6E3 !<correlations a partir de Heyberger>!		4.0E12	0.0
aC3H4+R11C2H5=C2H6+C3H3 19.8E3 !<asbutadiene>!		5.0E14	0.0
aC3H4+R10C2H3V=C2H4Z+C3H3 !<asbutadiene>!	5.0E14	0.0	19.8E3
!aC3H4+R4CH3=C4H7T !<Scherzer>!	5.7E10	0.0	6.8E3
!aC3H4+R4CH3=C4H7T !<Tsang91x2>!	3.4E11	0.0	7.4E3
!aC3H4+R4CH3=iC4H7 !<Tsang73>!	1.6E11	0.0	5.0E3
!aC3H4+R4CH3=C4H7T 7.4E3 !<Tsang91x2/4>!		0.8E11	0.0
aC3H4+R4CH3=iC4H7 !<Tsang73/3>!	0.4E11	0.0	5.0E3

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

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

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

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

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

!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+B1O=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+B1O=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+B1O=>CH2COZ+R1H+R4CH3	1.2E+5	2.56	-1130.0	
!<TSAnG91>! MF				
C3H6Y+B1O=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
B1O+C3H8=>R2OH+iC3H7	2.6E+0013	0.000	5200.0	! ME 15 CW
B1O+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

!*****

!*****

!*****!

! REACTIONS DES ESPECES NON OXYGENES EN C4 !
!*****!

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

R9C2H+R9C2H=C4H2	1.8E13	0.0	0.0
!<TSAng86>!			
2C2H2=C4H2+H2	1.5E13	0.0	42.7E3
!<LEUnG95>!			
C2H2+R9C2H=C4H2+R1H	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=1C6H4+R1H	29.6	3.33	9.6E3
!<WESTMORELAnD89, p=2.6kPa>!			
nC4H3+C2H2=1C6H4+R1H	2.77E-7	5.59	6.0E3
!<WESTMORELAnD89, p=101kPa>!			
!***			
!nC4H3+C2H2=1C6H5	1.73E11	-0.41	4.0E3
!<WESTMORELAnD89, p=2.6kPa>!			
nC4H3+C2H2=1C6H5	6.17E15	-1.51	4.8E3
!<WESTMORELAnD89, p=101kPa>!			
!***			
!nC4H3+C2H2=C6H5#	3.33E24	-3.89	9.2E3
!<WESTMORELAnD89, p=2.6kPa>!			
nC4H3+C2H2=C6H5#	7.0E14	-0.86	6.4E3
!<WESTMORELAnD89, p=101kPa>!			
!***			

!***** REACTIONS DE iC4H3 ***** (CH2//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+B1O=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=>1C6H5+R1H	6.0E12	0.0	0.0
!MILLER 92!			
!***** REACTIONS DE C4H4 ***** (CH2//CHC//CH) vinylacetylene *****!			
C3H3+B5CH2=C4H4+R1H	4.0E13	0.0	0.0
!<MILLER92>!			
R10C2H3V+C2H2=>C4H4+R1H	2.0E13	0.0	25.1E3
!(40,-40)<DOUTE95>!			
C4H4+R1H=>R10C2H3V+C2H2	2.0E13	0.0	12.4E3
!<DOUTE95>			
C2H4Z+R9C2H=C4H4+R1H	1.2E13	0.0	0.0
!(50,-50)<TSAnG86>!			
C4H4+R1H=nC4H3+H2	2.0E7	2.0	15.E3
!<Miller 92>!			
C4H4+R1H=iC4H3+H2	3.0E7	2.0	5.E3
!<Miller 92>!			
R9C2H+C4H4=>C2H2+iC4H3	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+B1O=aC3H4+B2CO	3.0E13	0.0	1.8E3
!<LEUnG95>!			
C4H4+B1O=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 1C6H6 n'intervient qu'ici

!nC4H5+C2H2=1C6H6+R1H 1.17E-15 7.84 2.0E3
!<WESTMOREELAnD89, p=2.6kPa>!

!nC4H5+C2H2=1C6H6+R1H 3.47E-15 7.73 2.5E3
!<WESTMOREELAnD89, p=101kPa>!

!***

!nC4H5+C2H2=C6H6#+R1H 1.90E7 1.47 4.2E3
!<WESTMOREELAnD89, p=2.6kPa>!

nC4H5+C2H2=C6H6#+R1H 2.38E8 1.18 3.7E3
!<WESTMOREELAnD89, p=101kPa>!

!***

!nC4H5+C2H2=1C6H7 8.74E12 -1.27 3.6E3
!<WESTMOREELAnD89, p=2.6kPa>!

nC4H5+C2H2=1C6H7 7.24E14 -1.38 4.0E3
!<WESTMOREELAnD89, p=101kPa>!

!***

!nC4H5+C2H2=C6H7# 1.96E19 -3.35 5.2E3
!<WESTMOREELAnD89, p=2.6kPa>!

nC4H5+C2H2=C6H7# 7.12E21 -3.64 6.3E3
!<WESTMOREELAnD89, p=101kPa>!

!***

!R10C2H3V+nC4H5=1C6H7+R1H 8.28E-28 11.89 5.0E3
!<WESTMOREELAnD89, p=2.6kPa>!

R10C2H3V+nC4H5=1C6H7+R1H 3.55E-43 16.16 -0.2E3
!<WESTMOREELAnD89, p=101kPa>!

!***

!R10C2H3V+nC4H5=1C6H8 2.90E15 -0.78 1.0E3
!<WESTMOREELAnD89, p=2.6kPa>!

R10C2H3V+nC4H5=1C6H8 1.50E13 -0.075 0.1E3
!<WESTMOREELAnD89, 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>!			
!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) *****stabililise 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) *****stabililise 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+B1O=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¥) *****stabililise 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 deduites de celles de C3H3

C4H5-2+B1O=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 !<TSAng86>!	5.0E11	0.0	7.3E3
C4H6Z2+R1H=nC4H5+H2 !<WAnG97>!	1.3E6	2.53	12.2E3
C4H6Z2+R1H=iC4H5+H2 !<WAnG97>!	6.6E5	2.53	9.2E3
C4H6Z2+R1H=C4H7-1 ESTIMATED *2!	2.6E13	0	3.2E3 !
C4H6Z2+R1H=C4H7Y ESTIMATED *2!	2.6E13	0	1.56E3 !
!C4H6Z2+R1H=C4H7-1 ESTIMATED	1.3E13	0	3.2E3 !
!C4H6Z2+R1H=C4H7Y ESTIMATED !	1.3E13	0	1.56E3 !
C4H6Z2+R4CH3=nC4H5+CH4 !<WU87>!	7.0E13	0.0	18.5E3
C4H6Z2+R4CH3=iC4H5+CH4 !<WU87-3kcal>!	7.0E13	0.0	15.5E3
C4H6Z2+R4CH3=C5H9Y 88 nist!	6.3E10	0.0	7.49E3 ! PERRIN
C4H6Z2+R4CH3=iC5H9 !Estimated*2!	1.8E11	0.0	8.0E3
!C4H6Z2+R4CH3=C5H9Y PERRIN 88 nist!	6.31E10	0.0	7.49E3 !
!C4H6Z2+R4CH3=iC5H9 !Estimated!	9.64E10	0.0	8.0E3
C4H6Z2+R10C2H3V=nC4H5+C2H4Z !<HIDAKA96>!	5.0E14	0.0	22.8E3
C4H6Z2+R10C2H3V=iC4H5+C2H4Z !<HIDAKA96-3kcal>!	5.0E14	0.0	19.8E3
C4H6Z2+B10=C3H5Y+R1H+B2CO !<LEUnG95,BREZInSKY84>!	6.0E08	1.45	0.9E3
!R10C2H3V+C4H6Z2=C6H8#+R1H !<frenklach >!	7.4E014	-0.66	8.42E3
!R10C2H3V+C4H6Z2=C6H8#+R1H !<WESTMORELAnD89, p=2.6kPa>!	2.28E12	-0.24	9.9E3
R10C2H3V+C4H6Z2=C6H8#+R1H !<WESTMORELAnD89, p=101kPa>!	4.15E-11	6.39	2.4E3
!*** !R10C2H3V+C4H6Z2=1C6H8+R1H !<WESTMORELAnD89, p=2.6kPa>!	1.0E10	1.05	14.0E3
R10C2H3V+C4H6Z2=1C6H8+R1H !<WESTMORELAnD89, p=101kPa>!	2.48E-15	8.20	6.3E3
!*** C4H6Z2+C2H2=C6H8# !<WESTMORELAnD89>!	2.3E12	0.0	35.0E3
!*** !MF car 1C6H9 n'intervient qu'ici !R10C2H3V+C4H6Z2=1C6H9 !<WESTMORELAnD89, p=2.6kPa>!	5.48E28	-5.31	9.3E3
!R10C2H3V+C4H6Z2=1C6H9 !<WESTMORELAnD89, p=101kPa>!	1.48E12	-0.17	3.2E3

!***			
!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+B1O=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+B1O=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+B1O=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 deduites 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
resonnance

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	6.0E+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>!				

! REACTIOs 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>!			


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!*****!
! 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)!

!*****!
! Amorcages 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

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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#+B1O=C5H7#+R2OH	2.6E13	0.0	5200	!BUDA05
C5H8#+B1O=C5H7#Y+R2OH	1.7E11	0.7	3250	
!HEYBERGER02				
C5H8#+B1O=C5H7#V+R2OH	1.2E11	0.7	7630	
!HEYBERGER02				

! Avec C2H5 !

C5H8#+R11C2H5=C5H7#+C2H6	2.0E11	0.0	11000	
!HEYBERGER02				
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/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#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(/ch2)/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=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			

!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!			

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!* MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE

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!* efficiency coefficients for O2, CO, CO2, H2O, AR, C6H6#

*!

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*****!

!* PRIMARY MECHANISM OF THE OXIDATION OF BENZENE

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

!REACTIONS OF BENZENE MOLECULES!

!***Umimolecular inititiation!

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

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

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

!***Bimolecular inititiation!

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

!***additions!

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

C6H6#+B1O=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#+B1O=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!

!REACTIONS OF C6H7# RADICALS!
 !***Isomerization!
 C6H7#=lC6H7 2.5E14 0.7 41.8E3
 !<WEISSMAN89!

!***Decomposition by beta-scission!
 !C6H7#=>C2H2+nC4H5 2.0E13 0.0 50.0E3
 !estimated!
 !Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
 HEYBERGER02!
 !***Oxidation!
 C6H7#+O2=C6H6#+R3OOH 7.9E11 0.0 9.9E3
 !estimated!
 !Oxidation of an allylic radical as proposed by HEYBERGER02!
 !combinations!
 C6H7#+R1H=C6H8# 1.0E14 0.0 0.0
 !estimated!
 !***Disproportionations!
 C6H7#+R1H=C6H6#+H2 3.3E12 0.0 0.0
 !<RISTORI01>!
 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 disproportionations ofC3H5Y proposed by TSANG91!

!REACTIONS OF C6H5# RADICALS!
 !***Isomerization!
 C6H5#=lC6H5 5.0E13 0.0 72.5E3
 !<BRAUN89>!
 !lC6H5 = ch///c/ch//ch/ch//ch(.)!
 lC6H5=>2C2H2+R9C2H 2.0E13 0.0 51.0E3
 !estimated!
 !DH298 =44kcal/mol, Eadd=7 kcal/mol!
 lC6H5=lC6H4+R1H 2.0E12 0.0 41.0E3
 !estimated!
 !lC6H4 = 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#+B1O 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#+B1O=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>!
!***disproportionations!
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!

!MF
C6H5O2+R3OOH=C6H5OOH+O2 2.0E11 0.00 -1300
C6H5OOH=C6H5O#+R2OH 1.5E16 0.00 43000

!REACTIONS OF PHENOXY RADICALS!
!***CO elimination!
C6H5O#=B2CO+C5H5# 2.5E11 0.0 43.8E3
!<BAULCH92>!
!***Combinations!
!--C6H5O#+R1H(+M)=C6H5OH#(+M) 2.5E14 0.0 0.0
!<FRENKLACH>!
C6H5O#+R1H(+M)=C6H5OH#(+M) 1.0E14 0.0 0.0
!estimated!

LOW /1.0E94 -21.84 13.9E3/
!<FRENKLACH>!

TROE /0.043 304 60000 5896/
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
C6H5O#+R1H=C5H6#+B2CO 1.1E53 -10.7 41.4E3
!<TAN96>!

C6H5O# + B1O = OC6H4OH	2.6E10	0.47	0.8E3
!<LIN95>!			
C6H5O# + B1O = OC6H4O + R1H	8.5E13	0.0	0.0
!<FRANCK94>!			
C6H5O# + B1O = C5H5# + CO2	1.0E13	0.0	0.0
!<FRANCK94>!			
!REACTIONS OF HYDROXYPHENOXY RADICALS!			
!***CO elimination!			
OC6H4OH = B2CO + C5H4OH#	7.4E11	0.0	43.8E3
!estimated!			
!as for phenoxy radicals!			
!REACTIONS OF CYCLOPENTADIENYL RADICALS!			
!***Isomerization!			
C5H5# = 1C5H5	1.0E14	0.0	45.5E3
!<BRAUN89>!			
!1C5H5 = ch///c/ch//ch/ch2(.), DH298 = 31kcal/mol!			
!MF car 1C5H6 n'intervient qu'ici			
!1C5H5 + R1H = 1C5H6	1.0E14	0.0	0.0
!estimated!			
1C5H5 = C3H3 + C2H2	2.0E13	0.0	50.0E3
!estimated!			
!DH298 = 43kcal/mol, Eadd = 7 kcal/mol!			
!***Reactions with O2!			
C5H5# + O2 = R5CHO + C4H4O	1.2E19	-2.48	11.0E3
!<ZHONG98>!			
!***Combinations!			
C5H6# = C5H5# + R1H	5.0E15		0.00
7.87E4	! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>		
C5H5# + B1O = C5H4O# + R1H	5.8E13	-0.02	0.02E3
!<ZHONG98>!			
C5H5# + B1O => 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!			
!***disproportionations!			
C5H5# + R3OOH => C5H6# + O2	2.5E9	1.0	3.5E3
!estimated!			
!estimated as for allylic radicals (HEYBERGER02)/10!			
!REACTIONS OF CYCLOPENTADIONYL RADICALS!			

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!***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 disproportionations considered!

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!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#+B1O=CO2+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!

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

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!REACTIONS OF PHENOL AND DERIVED RADICALS!
C6H5OH#=C5H6#+B2CO           1.0E12      0.0      61.2E3
!<HORN98>!

C6H5OH#+O2=R3OOH+C6H5O#      1.0E13      0.0      38.9E3
!<ALZUETA00>!

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C6H5OH#+B1O=OC6H4OH+R1H !estimated!	1.6E13	0.0	3.4E3	
!as the addition of O-atoms to toluene (DACOSTA01)!				
C6H5OH#+R1H=C6H5O#+H2 !<ALZUETA00>!	1.2E14	0.0	12.4E3	
C6H5OH#+B1O=C6H5O#+R2OH !<ALZUETA00>!	1.3E13	0.0	2.9E3	
C6H5OH#+R2OH=C6H5O#+H2O !<SHANDROSS96>!	1.4E8	1.4	-0.96E3	
C6H5OH#+R3OOH=C6H5O#+H2O2 !<ALZUETA00>!	1.0E12	0.0	10.0E3	
C6H5OH#+R4CH3=C6H5O#+CH4 !<MULCAHY65>!	1.8E11	0.0	7.7E3	
C6H5OH#+C6H5#=C6H5O#+C6H6# !<ALZUETA00>!	4.9E12	0.0	4.4E3	
!C6H5OH#+C5H5#=C6H5O#+C5H6# !estimated!	4.9E11	0.0	9.4E3	
!C6H5OH#+C3H5Y=C6H5O#+C3H6Y !estimated!	4.9E11	0.0	9.4E3	
!C6H5OH#+iC4H5=C6H5O#+C4H6Z2 !estimated!	4.9E11	0.0	9.4E3	
C6H5OH#+C5H5#=C6H5O#+C5H6# !mf <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	
C6H5OH#+C3H5Y=C6H5O#+C3H6Y !mf <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	
C6H5OH#+iC4H5=C6H5O#+C4H6Z2 !mf <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	
!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!				
C6H5OH#+R1H=C6H4OH#+H2 !<SHANDROSS96>!	1.7E14	0.0	16.0E3	
C6H5OH#+B1O=C6H4OH#+R2OH !estimated!	2.0E13	0.0	14.7E3	
C6H5OH#+R2OH=C6H4OH#+H2O !<SHANDROSS96>!	1.4E13	0.0	4.6E3	
C6H5OH#+R3OOH=C6H4OH#+H2O2 !estimated!	4.0E11	0.0	28.9E3	
C6H5OH#+R4CH3=C6H4OH#+CH4 !estimated!	2.0E12	0.0	15.0E3	
!as the H-abstractions from benzene!				
C6H4OH#+O2=OC6H4OH+B1O !estimated!	2.1E13	0.0	6.1E3	
!as for phenyl radicals (FRANCK94)!				
C6H4OH#+R1H=C6H5OH# !estimated!	1.0E14	0.0	0.0	
C6H4OH#+R4CH3=HOC6H4CH3	5.0E12	0.0	0.0	!mf
!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!				
C5H6#+O2=>C5H5#+R3OOH !<INGHAM94>!	1.4E12	0.0	31.6E3	
!C5H6#+R1H=C5H7# !estimated!	5.2E13	0.0	3.2E3	
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!				

C5H6#+B1O=>C5H5O#+R1H !<ZHONG98>!	8.9E12	-0.15	590.0	
C5H6#+R1H=C5H5#+H2 !<ROY97>!	2.8E13	0.0	2.0E3	
C5H6#+B1O=C5H5#+R2OH !<ZHONG98>!	4.8E4	2.7	1.1E3	
C5H6#+R2OH=C5H5#+H2O !<ZHONG98>!	3.1E6	2.0	0.0	
C5H6#+R3OOH=C5H5#+H2O2 !<ZHONG98>!	1.1E4	2.6	12.9E3	
C5H6#+R4CH3=C5H5#+CH4 !<ZHONG98>!	1.8E-1	4.0	0.0	
C5H6#+C3H5Y=C5H5#+C3H6Y !astoluene!	1.6E12	0.0	15.1E3	
C5H6#+nC4H5=C5H5#+C4H6Z2 !astoluene!	1.6E12	0.0	11.1E3	
C5H6#+iC4H5=C5H5#+C4H6Z2 !astoluene!	1.6E12	0.0	15.1E3	
!C5H6#+C3H5Y=C5H5#+C3H6Y !estimated!	6.0E12	0.0	0.0	
!C5H6#+nC4H5=C5H5#+C4H6Z2 !estimated!	6.0E12	0.0	0.0	
!C5H6#+iC4H5=C5H5#+C4H6Z2 !<EMDEE92>!	6.0E12	0.0	0.0	
 !C5H7#=>C2H2+C3H5Y !estimated!	2.0E13	0.0	35.5E3	
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by HEYBERGER02!				
!C5H7#+O2=C5H6#+R3OOH !estimated!	7.9E11	0.0	5.0E3	
!oxidation of an alkylic radical!				
 !REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!				
C5H4O#=>2C2H2+B2CO !<ALZUETA00>!	5.7E32	-6.76	68.5E3	
!C5H4O#=B2CO+C4H4 roda PENGLOAN!	1.00e12	0.0	53000	!
C5H4O#+R1H=B2CO+nC4H5 !estimated!	2.6E13	0.0	3.2E3	
 !estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!				
C5H4O#+B1O=C4H4+CO2 !<ALZUETA00>!	1.0E13	0.0	2.0E3	
C5H4O#+R1H=C5H3O#+H2 idem C6H6#+R1H=C6H5#+H2	8.13E7	2.031	15.88E3	!MF
C5H4O#+B1O=C5H3O#+R2OH !<ALZUETA00>!	1.4E13	0.0	14.7E3	
C5H4O#+R2OH=C5H3O#+H2O !<ALZUETA00>!	1.1E8	1.42	1.4E3	
 C5H3O#=>C2H2+B2CO+R9C2H !estimated!	2.0E13	0.0	51.0E3	
!estimated as the decomposition of 1C6H5!				
C5H3O#+O2=>CO2+C2H2+R12CHCOZ !<ALZUETA00>!	9.7E58	-13.47	38.2E3	

C5H5OH#+R1H=C5H5O#+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	!* *! *! *!
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!* 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+B1O=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+B1O=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 1.02E4 2.5 12339.3
!PITZ

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+B1O 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+B1O	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 x rpd x 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 disproportionation 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')>!
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!(h') : Rate constant of the isomerisation :!

! 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>!

!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>

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

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```

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

```

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

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```

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

```

!HOC6H4CH2+B1O=C6H4OH#+HCHO 8E13 0.0 0.0

```

```

! metatheses
HOC6H4CH3+R1H=OC6H4CH3+H2      1.2E14      0.0      12.4E3
      !<estimated(s)>!
HOC6H4CH3+B1O=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+B1O=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)>!			
HOC6H4CH3+C6H5CH2OO=HOC6H4CH2+C6H5CH2OOH	4.0E11	0.0	14.0E3
!<estimated(t)>!			
HOC6H4CH3+C6H5CH2O=HOC6H4CH2+C6H5CH2OH	1.6E11	0.0	11.1E3
!<estimated(t)>!			
HOC6H4CH2+O2=HOC6H4CH2OO	4.6E11	0.0	-377.0
!<estimated(u)>!			
HOC6H4CH2+O2=HOC6H4CH2O+B1O	6.3E12	0.0	40.0E3
!<estimated(u)>!			
HOC6H4CH2+R3OOH=HOC6H4CH2O+R2OH	5.0E12	0.0	0.0
!<estimated(u)>!			
!(u) : Rate constant taken equal to that of the same reaction for benzyl radicals !			
HOC6H4CH2+R1H=HOC6H4CH3	1.0E14	0.0	0.0
!<estimated(g)>!			
HOC6H4CH2+R4CH3=C6H5OH#+C2H4Z	5.0E12	0.0	0.0
!<estimated(g)>!			
HOC6H4CH2OO=C6H4OHCHO+R2OH	3.4E9	1.0	37.5E3
!<estimated(v)>!			
!(v) : Rate constant taken equal to that of the same reaction for benzyl peroxy radicals !			
HOC6H4CH2O=R1H+C6H4OHCHO	2.0E13	0.0	27.5E3
!<estimated(w)>!			
HOC6H4CH2O=C6H4OH#+HCHO	2.0E13	0.0	27.5E3
!<estimated(w)>!			
HOC6H4CH2O+O2=R3OOH+C6H4OHCHO	6.0E10	0.0	1.6E3
!<estimated(w)>!			
!(w) : Rate constant taken equal to that of the same reaction for benzyl alcoxy radicals !			

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

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

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

C6H5CH2OH+O2=R3OOH+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 0.08.1E3 !<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. 36.373E3 !MF
DHR=36.79 correlation baptiste E=0.6*DHR+14.3

!R15C2H5O=CH3CHO+R1H 2.0E14 0. 23.3E3 !(243,-
243)<HEICKLEN88NIST>!

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

!** 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 7.2E8 1.5 6.79E3 !MF

correlation Dean-Bozzelli 2000

etC6H5+B1O=C8H9#-1+R2OH 5.1E8 1.5 5.05E3

!MF correlation Dean-Bozzelli 2000


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etC6H5+R2OH=C8H9#-1+H2O          3.6E6          2.0          4.82E2          !MF
correlation Dean-Bozzelli 2000
etC6H5+R3OOH=C8H9#-1+H2O2      4.2E4          2.69 1.85E4          !MF
correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4      2.43E6          1.87 1.03E4          !MF correlation
Dean-Bozzelli 2000

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

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

! Ajout ipso MF
etC6H5+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>

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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.

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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+B1O=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	
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! 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+B1O=>C6H4CH3+C6H5CHO+R2OH      10.5E11      0.0
0.0 ! 5/3 as toluene

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!*****!

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!*REACTIONS OF PhenolCH2bz *!

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!*****!

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!Ajout Ipso MF negligeable
!C6H5OH#+benzyl=PhenolCH2bz+R1H      1.0E12      0.0
0.00 !
!HOC6H4CH2+C6H6#=PhenolCH2bz+R1H      1.0E12      0.0      0.00
!

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```

! ajout MF
C6H4OH#+benzyl=PhenolCH2bz      1.0E13      0.0
0.00 !
HOC6H4CH2+C6H5#=PhenolCH2bz      1.0E13      0.0
0.00 !

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```

! ajout MF
PhenolCH2bz+R1H=>C6H5O#+C4H2+pC3H4+H2      2.92E6      2.372
5.81E3 !AS TOLUENE
PhenolCH2bz+B1O=>C6H5O#+C4H2+pC3H4+R2OH      6.3E11      0.0      0.0
!AS TOLUENE
PhenolCH2bz+R2OH=>C6H5O#+C4H2+pC3H4+H2O      5.2E09      1.0
0.87E3 !AS TOLUENE

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!*****!

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!*REACTIONS OF PhenolC2H4bz *!

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!*****!

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```

!Ajout Ipso MF
! negligeable 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+C6H5O#+H2O      8.75E09      1.0
0.87E3 ! 5/3 as toluene
PhenolC2H4bz+R1H=>styrene+C6H5O#+H2      4.875E6      2.372
5.81E3 ! 5/3 as toluene
PhenolC2H4bz+B1O=>styrene+C6H5O#+R2OH      10.5E11      0.0      0.0
! 5/3 as toluene

```

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!*****!

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```

!*REACTIONS OF Benzaldtol *!

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!*****!

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!Ajout Ipso MF negligeable

```

!C6H5CO+HOC6H4CH3=BenzaIdtol+R1H

! ajout MF

C6H5CO+OC6H4CH3=BenzaIdtol 3.0E12 0.0
0.00 !

! ajout MF

BenzaIdtol+R2OH=>C6H5CHO+C6H5CO+H2O 5.2E09 1.0
0.87E3 !AS TOLUENE
BenzaIdtol+R1H=>C6H5CHO+C6H5CO+H2 2.92E6 2.372 5.81E3
!AS TOLUENE
BenzaIdtol+B1O=>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+B1O=>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+B1O=>B2CO+C6H5O#+R2OH 6.0E12 0.0 1.8E3 !AS
C6H5CHO
DUP

!*****!

!*REACTIONS OF C6H5C4H7 *!

!*****!

benzyl+C3H5Y=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+B1O=>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+B1O=>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#+B1O=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#+B1O=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+B1O=>C6H5CO+B2CO+R1H 6.00E4 2.56 -1.13E3

```

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

```

```

naphthalene+O2=R3OOH+naphthyl  8.0E13          0.0          63.4E3
!like benzene <ALZUETA00>A*8/6!
naphthalene+B10=>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+B10=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+B10   2.6E13   0.0   6.1E3  !as n-
buthylbenzene
naphthyl+B10=>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 4.3E12  0.0  4.89E3 !in Slavinskaya09
A/10

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```

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

```

```

indene+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+B1O=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  75.0E3  !Slavinskaya09
5.0E13  0.0  37.5E3
indenyl+R1H=indene                1.0E14  0.0  0.0     !as n-buthylbenzene
C6H5#+C3H3=indene                6.46E12  0.0  0.0     !Slavinskaya09
indenyl+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+B1O=>C6H6#+B2CO+R9C2H    5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H
indenyl+B1O=>C6H5#C2H+R5CHO      5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=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
B1O+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+B1O=>R2OH+CH3styre+R1H				
Touchard!	3.4E+10	0.7	1.33E3	!
!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+B1O=>R2OH+CH3styre+R1H				
toluene A/3	2.1E+11	0.0	0	! as
cumene+R1H=>H2+CH3styre+R1H				
toluene A/3	0.97E+06	2.372	5.81E3	! as
cumene+R2OH=>H2O+CH3styre+R1H				
toluene A/3	1.73E+09	1.0	0.87E3	! as
cumene+R3OOH=>H2O2+CH3styre+R1H				
toluene A/3	1.33E+11	0.0	14.0E3	! as
cumene+R4CH3=>CH4+CH3styre+R1H				
A/3	1.3	3.76	6.98E3	! as toluene
C9H11#-1=styrene+R4CH3				
	2.0E+13	0.0	31.0E3	! Touchard!
C9H11#-1=C3H6Y+C6H5#				
EvansPolani corr (Ea=18.9+0.53drH)!	2.0E+13	0.0	38.5E3	!Beta-sciss
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				
addition	5.8E13	0.0	8.1E3	!ipso-
!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				
!estimated (analogie etC6H5)!	1.2E13	0.0	49.0E3	
!**METATHESES-Decompositions				

B1O+CH3styre=>R2OH+aC3H4+C6H5# Touchard	5.1E+13	0.0	7.85E3	!
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 mechanism	4.0E13	0.0	4.2E3	!Butane
C6H5CH2CHO+R2OH=>H2O+B2CO+benzyl mechanism	4.2E12	0.0	0.5E3	!Butane
C6H5CH2CHO+R3OOH=>H2O2+B2CO+benzyl !Butane mechanism	1.0E12	0.0	10.0E3	
C6H5CH2CHO+R4CH3=>CH4+B2CO+benzyl mechanism	2.0E-6	0.0	2.5E3	!Butane
C6H5CH2CHO+R11C2H5=>C2H6+B2CO+benzyl mechanism	1.3E12	0.0	8.5E3	!Butane

!*****!
!* 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# !exgas	6.0E11	0.0	17000	
C6H5COCH3+R4CH3=>CH4+CH2COZ+C6H5#	3.0E-1	4.0	8200	!exgas
!C6H5COCH3+R11C2H5=>C2H6+CH2COZ+C6H5#	3E11	0.0	13500	!exgas

!!
! Reactions of chlorinated compounds !
!!
!

!Reactions for H/CL system (Pelucchi et al., 2016)
R1H+CL+M=HCL+M 2.0E+23 -2.45 0.0! Schading
and Roth, 1994
H2/2.0/ CL2/2.0/ N2/2.0/
CL+H2=HCL+R1H 9.5E+07 1.72 3060 !
Kumaran et al., 1994
CL2+M=CL+CL+M 5.7E+15 0.00 55596 ! Leylegian et
al., 2005
H2/2.0/ CL2/6.9/ N2/2.0/
CL2+R1H=HCL+CL 8.6E+13 0.00 1172.0 !
Baulch et al., 1981

!Reactions for PHICL

!unimolecular initiations
PHICL=C6H5#+CL 3.0E+15 0 95.6E+3 !Ritter et
al., 1990 meilleur résultat

!Molecular reaction
 PHICL+H2<=>C6H6#+HCL 1.3605E+06 2.18
 73174.0 !calculated, see work

!ipso-additions

PHICL+R1H=C6H6#+CL 4.26E+07 1.772 7.951E+03
 !calculated, see work
 PHICL+CL=PHI12CL2+R1H 1.17E+04 2.992 22.576E+03
 !calculated, see work
 PHICL+CL=PHI13CL2+R1H 8.57E+03 3.057 21.927E+03
 !calculated, see work
 PHICL+CL=PHI14CL2+R1H 5.48E+03 3.027 21.829E+03
 !calculated, see work
 PHICL+C6H5#=BPNL3CL+R1H 1.264E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 PHICL+C6H5#=BPNL4CL+R1H 0.632E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 PHICL+C6H5#=BPNL2CL+R1H 1.264E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 PHICL+C6H5#=biphenyl+CL 5.6E+12 -0.074 7.5E+3
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R2PHICL+C6H6#=BPNL2CL+R1H 5.6E+12 -0.074 7.5E+3
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R3PHICL+C6H6#=BPNL3CL+R1H 5.6E+12 -0.074 7.5E+3
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R4PHICL+C6H6#=BPNL4CL+R1H 5.6E+12 -0.074 7.5E+3
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R4PHICL+PHICL=BB44CL2+R1H 3.16E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R4PHICL+PHICL=BB43CL2+R1H 6.32E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R4PHICL+PHICL=BB42CL2+R1H 6.32E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R3PHICL+PHICL=BB33CL2+R1H 6.32E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R3PHICL+PHICL=BB32CL2+R1H 6.32E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 R2PHICL+PHICL=BB22CL2+R1H 6.32E+12 0.000 8.505E+03
 !estimated as C6H6#+C6H5#=biphenyl+R1H Wang et al., 1997
 PHICL+R4CH3=toluene+CL 1.20E+12 0.0 15774
 !estimated as C6H6#+R4CH3=toluene+H Robaugh et al., 1986

!H-atom abstractions

PHICL+R1H=R2PHICL+H2 1.4947E+08 1.79 12328
 !Calculated, see work
 PHICL+R1H=R3PHICL+H2 1.2290E+08 1.81 10930
 !calculated, see work
 PHICL+R1H=R4PHICL+H2 1.3526E+08 1.81 11748
 !calculated, see work
 PHICL+CL=R2PHICL+HCL 1.4947E+08 1.79 12328
 !estimated H-abstraction
 PHICL+CL=R3PHICL+HCL 1.2290E+08 1.81 10930
 !estimated H-abstraction
 PHICL+CL=R4PHICL+HCL 1.3526E+08 1.81 11748
 !estimated H-abstraction
 PHICL+C6H5#=R2PHICL+C6H6# 1.4947E+08 1.79 12328
 !estimated H-abstraction

PHICL+C6H5#=R3PHICL+C6H6#	1.2290E+08	1.81	10930	
!estimated H-abstraction				
PHICL+C6H5#=R4PHICL+C6H6#	1.3526E+08	1.81	11748	
!estimated H-abstraction				
!Cl-atom abstractions				
PHICL+CL=C6H5#+CL2	2.34E+09	1.743	12.484E+03	!estimated
PHICL+R1H=C6H5#+HCL	1.608E+09	1.57	10988	
!calculated, see work				
!Terminations				
C6H5#+R2PHICL=BPNL2CL	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
C6H5#+R3PHICL=BPNL3CL	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
C6H5#+R4PHICL=BPNL4CL	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R4PHICL+R4PHICL=BB44CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R4PHICL+R3PHICL=BB43CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R4PHICL+R2PHICL=BB42CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R3PHICL+R3PHICL=BB33CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R3PHICL+R2PHICL=BB32CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
R2PHICL+R2PHICL=BB22CL2	1.55E+14	-0.45	-550.0	!estimated
as C6H5#+C6H5#=biphenyl Tranter et al., 2010				
!Recalculated				
C6H5#+H2<=>C6H6#+R1H			5.0209E+11	-.14
2748.9 !calculated, see work				

END