```
!*****************************************************************************
*
!
!
!                      DEPARTEMENT DE CHIMIE PHYSIQUE DES REACTIONS
!
!                                  ENSIC-CNRS                                 !
!                            1 RUE GRANDVILLE, BP 451
!
!                           54001 NANCY CEDEX - FRANCE
!
!
!
!*****************************************************************************
*
!
!
!             LOW and  HIGH TEMPERATURE MECHANISM FOR THE OXIDATION
!
!                       OF N-HEPTANE, ETBE, MTBE MIXTURE
!
!                      FILE USABLE BY CHEMKIN II (SANDIA)
!
!             AUTHORS : P.A. Glaude, R. Fournet, V. Warth, F. Battin-Leclerc
!
!                                 G.M. Come and G. Scacchi
!
!                                   18 january 2002
!
!
!
!*****************************************************************************
*!
ELEMENTS
ELEMENTS
H O C N HE
END
SPECIES

! Biradicals :
B1O
B2CO
B3C
B4CH
B5CH2
B6CH2


! Primary molecules :
H2
H2O
O2
H2O2
CH4
HCHO
CH3OH
CO2
CH3O2H
C2H2
C2H4Z
C2H6
CH2COZ
CH3CHO
C2H5OH
```

C2H5O2H
CH3COO2H
C3H6Y
C3H8
C4H8Y
C4H10
C2H5CHO
C3H7OH
C2H6CO
C3H8CO
C4H6Z2
C7H16
C5H12O
C6H14O
C5H10Z
C6H12Z
C4H8OY
C5H10OY
C3H5OOHY
C6H11OOHZ
C7H14Z
C4H7OOHY
C5H9OOHZ
C4H7OOOHY
C5H9OOOHY
C6H12OZ
C3H7CHO
C6H14CO
C4H9CHO
C6H13CHO
C4H9OCHO
C5H11OCHO
C2H5COOOH
C5H12OCO
C2H4CHOOOH
C3H6CHOOOH
C6H13COOOH
C6H12CHOOOH
C4H8OCHOOOH
C5H10OCHOOOH
C5H11OCOOOH
C3H7COOOH
C4H8CHOOOH
C4H9COOOH
C4H10CO
C2H4COO4H2
C3H4OHOOHZ
C3H5OHY
C4H9OCOOOH
C4H6O4H2Y
C3H5OHCHOOOH
C3H6OHCHO
C4H9OH
C4H9OOH
C3H7OOH
C5H12
C5H11OH
C4H10O
C6H14
C8H18
C7H15OOH
C5H11OOOH
C6H13OOOH
C5H11OOH

C4H8OHOOH

! Secondary molecules :
C4H7OHY
C4H6YZ
C5H9OHZ
C5H8Z2
C5H11CHO
C6H11OHZ
C6H10Z2
C3H7COOH
C2H5COOH
C3H5CHOY
C6H10Y2
C7H12Y2
C8H14Y2
C4H7CHOY
C9H16Y2
C5H9CHOY
C10H18Y2

! Cyclic primary molecules :

! Cyclic secondary molecules :
C2H4O#3
C3H6O#3
C3H6O#4
C4H8O#3
C4H8O#4
C4H8O#5
C7H14O#3
C7H14O#4
C7H14O#5
C7H14O#6
C5H10O2#4
C6H12O2#4
C6H12O2#5
C6H12O2#3
C5H10O#3
C5H10O#4
C5H10O#5
C5H10O#6
C3H5O#3OOH
C3H5O#4OOH
C4H7O#3OOH
C4H7O#4OOH
C4H7O#5OOH
C7H13O#3OOH
C7H13O#4OOH
C7H13O#5OOH
C7H13O#6OOH
C5H9O2#4OOH
C6H11O2#4OOH
C6H11O2#5OOH
C6H11O2#3OOH
C5H9O#3OOH
C5H9O#4OOH
C5H9O#5OOH
C5H9O#6OOH
C4H8O2#4
C4H7O2#4OOH
C2H3O#4COOOH
C3H5O#4COOOH
C3H5O#5COOOH

C6H11O#4COOOH
C6H11O#5COOOH
C6H11O#6COOOH
C4H7O#4COOOH
C4H7O#5COOOH
C4H7O#6COOOH
C6H10#ZZ2
C7H12#ZZ2
C8H14#ZZ2
C6H12O#3

! Free radicals :
R1H
R2OH
R3O2H
R4CH3
R5CHO
R6CH2OH
R7CH3O
R8CH3OO
R9C2H
R10C2H3V
R11C2H5
R12CHCOZ
R13CH2CHO
R14CH3CO
R15C2H5O
R16C2H4O2H
R17C2H5OO
R18CH3COOO
R19C3H7
R20C4H9
R21C7H15
R22C7H15
R23C7H15
R24C7H15
R25C5H11O
R26C5H11O
R27C6H13O
R28C6H13O
R29C6H13O
R30C3H7OO
R31C4H9OO
R32C7H15OO
R33C7H15OO
R34C7H15OO
R35C7H15OO
R36C5H11
R37C5H11OOO
R38C5H11OOO
R39C4H9
R40C6H13OOO
R41C6H13OOO
R42C6H13OOO
R43C4H9O
R44C3H6OOH
R45C3H6OOH
R46C4H8OOH
R47C4H8OOH
R48C4H8OOH
R49C7H14OOH
R50C7H14OOH

R51C7H14OOH
R52C7H14OOH
R53C7H14OOH
R54C7H14OOH
R55C7H14OOH
R56C7H14OOH
R57C7H14OOH
R58C7H14OOH
R59C7H14OOH
R60C7H14OOH
R61C7H14OOH
R62C7H14OOH
R63C7H14OOH
R64C7H14OOH
R65C7H14OOH
R66C7H14OOH
R67C5H11OO
R68C5H11
R69C5H10OOOH
R70C5H10OOOH
R71C5H10OOOH
R72C4H9OO
R73C6H12OOOH
R74C6H12OOOH
R75C6H12OOOH
R76C6H12OOOH
R77C6H12OOOH
R78C6H12OOOH
R79C6H12OOOH
R80C3H6OOOOH
R81C3H6OOOOH
R82C4H8OOOOH
R83C4H8OOOOH
R84C4H8OOOOH
R85C4H8OOH
R86C7H14OOOOH
R87C7H14OOOOH
R88C7H14OOOOH
R89C7H14OOH
R90C5H10OOH
R91C7H14OOOOH
R92C7H14OOOOH
R93C5H10OOH
R94C7H14OOOOH
R95C7H14OOOOH
R96C3H6OOH
R97C7H14OOOOH
R98C7H14OOH
R99C4H8OOH
R100C7H14OOOOH
R101C5H10OOH
R102C7H14OOOOH
R103C7H14OOH
R104C7H14OOOOH
R105C7H14OOOOH
R106C7H14OOOOH
R107C7H14OOH
R108C3H6OOH
R109C7H14OOOOH
R110C4H8OOH
R111C7H14OOOOH
R112C7H14OOH
R113C7H14OOH
R114C7H14OOOOH

R115C7H14OOOOH
R116C7H14OOH
R117C7H14OOOOH
R118C5H10OOH
R119C5H10OOH
R120C5H10OOH
R121C5H10OOH
R122C5H11OO
R123C5H10OOOOOH
R124C5H10OOOOOH
R125C5H10OOOH
R126C4H8OOH
R127C5H10OOOOOH
R128C5H10OOOH
R129C4H8OOH
R130C6H12OOOOOH
R131C6H12OOOOOH
R132C6H12OOOH
R133C6H12OOOOOH
R134C4H8OOOH
R135C6H12OOOOOH
R136C6H12OOOOOH
R137C6H12OOOH
R138C6H12OOOOOH
R139C6H12OOOOOH
R140C6H12OOOH
R141C3H5O4H2
R142C3H5O4H2
R143C3H6OOOOH
R144C3H5O4H2
R145C3H5O4H2
R146C4H7O4H2
R147C4H8OOOOH
R148C4H7O4H2
R149C4H7O4H2
R150C4H7O4H2
R151C4H7O4H2
R152C4H7O4H2
R153C4H8OOOOH
R154C4H7O4H2
R155C4H7O4H2
R156C4H8OOOOH
R157C7H13O4H2
R158C7H13O4H2
R159C7H13O4H2
R160C7H13O4H2
R161C7H13O4H2
R162C7H13O4H2
R163C7H13O4H2
R164C7H13O4H2
R165C7H13O4H2
R166C7H13O4H2
R167C7H13O4H2
R168C7H13O4H2
R169C7H13O4H2
R170C7H13O4H2
R171C7H13O4H2
R172C7H14OOOOH
R173C5H10OOOOH
R174C5H10OOH
R175C5H10OOH
R176C7H13O4H2
R177C7H13O4H2
R178C7H13O4H2

R179C7H13O4H2
R180C7H13O4H2
R181C7H13O4H2
R182C7H13O4H2
R183C7H13O4H2
R184C7H13O4H2
R185C5H10OOOOH
R186C7H13O4H2
R187C7H13O4H2
R188C7H13O4H2
R189C7H13O4H2
R190C7H13O4H2
R191C3H6OOOOH
R192C7H13O4H2
R193C7H13O4H2
R194C7H13O4H2
R195C7H13O4H2
R196C7H13O4H2
R197C7H14OOOOH
R198C4H9OO
R199C7H13O4H2
R200C7H13O4H2
R201C7H13O4H2
R202C7H13O4H2
R203C5H10OOOOH
R204C5H11OO
R205C5H10OOH
R206C7H13O4H2
R207C7H13O4H2
R208C7H13O4H2
R209C7H13O4H2
R210C7H14OOOOH
R211C7H13O4H2
R212C7H13O4H2
R213C7H13O4H2
R214C7H13O4H2
R215C7H13O4H2
R216C7H13O4H2
R217C7H14OOOOH
R218C3H7OO
R219C7H13O4H2
R220C7H13O4H2
R221C7H13O4H2
R222C7H13O4H2
R223C7H13O4H2
R224C7H13O4H2
R225C7H14OOOOH
R226C7H14OOOOH
R227C7H13O4H2
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R231C7H13O4H2
R232C7H13O4H2
R233C7H14OOOOH
R234C7H13O4H2
R235C7H13O4H2
R236C7H13O4H2
R237C5H10OOOOH
R238C5H10OOOOH
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R241C5H10OOH
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R244C5H9O4H2
R245C5H9O4H2
R246C5H9O4H2
R247C5H10OOOOOH
R248C4H8OOOOH
R249C4H9OO
R250C5H9O4H2
R251C5H10OOOOOH
R252C4H8OOOOH
R253C6H11O4H2
R254C6H11O4H2
R255C6H11O4H2
R256C6H11O4H2
R257C6H11O4H2
R258C6H11O4H2
R259C6H11O4H2
R260C6H12OOOOOH
R261C6H11O4H2
R262C6H11O4H2
R263C6H11O4H2
R264C4H8OHOO
R265C6H11O4H2
R266C6H11O4H2
R267C6H11O4H2
R268C6H12OOOOOH
R269C6H11O4H2
R270C6H11O4H2
R271C6H12OOOOOH
R272C3H5O4H2
R273C4H7O4H2
R274C4H7O4H2
R275C4H7O4H2
R276C4H7O4H2
R277C4H7O4H2
R278C5H9O4H2
R279C5H9O4H2
R280C7H13O4H2
R281C7H13O4H2
R282C7H13O4H2
R283C5H9O4H2
R284C5H9O4H2
R285C5H9O4H2
R286C5H9O4H2
R287C5H10OOOOH
R288C5H10OOOOH
R289C5H10OOH
R290C4H7O4H2
R291C5H9O4H2
R292C5H9O4H2
R293C5H9O4H2
R294C5H9O4H2
R295C5H9O4H2
R296C3H5O4H2
R297C3H5O4H2
R298C7H13O4H2
R299C7H13O4H2
R300C7H13O4H2
R301C7H13O4H2
R302C7H13O4H2
R303C7H13O4H2
R304C4H8OOH
R305C4H9
R306C5H9O4H2

R307C5H9O4H2
R308C5H9O4H2
R309C5H9O4H2
R310C5H11
R311C5H10OOOOH
R312C7H13O4H2
R313C7H13O4H2
R314C7H13O4H2
R315C7H13O4H2
R316C7H13O4H2
R317C5H9O4H2
R318C5H9O4H2
R319C5H9O4H2
R320C7H13O4H2
R321C7H13O4H2
R322C7H13O4H2
R323C7H13O4H2
R324C7H13O4H2
R325C3H7
R326C7H13O4H2
R327C7H13O4H2
R328C7H13O4H2
R329C7H13O4H2
R330C5H9O4H2
R331C7H13O4H2
R332C7H13O4H2
R333C7H13O4H2
R334C7H13O4H2
R335C5H9O4H2
R336C5H9O4H2
R337C5H9O4H2
R338C5H9O4H2
R339C5H9O4H2
R340C5H10OOOOH
R341C4H7O4H2
R342C5H9OO4H2
R343C5H9OO4H2
R344C4H7O4H2
R345C4H7O4H2
R346C4H8OOH
R347C4H9
R348C5H9OO4H2
R349C4H7OO4H2
R350C6H11OO4H2
R351C6H11OO4H2
R352C6H11OO4H2
R353C4H7OHOOH
R354C4H8OH
R355C6H11OO4H2
R356C6H11OO4H2
R357C6H11OO4H2
R358C6H11OO4H2
R359C4H7O4H2
R360C5H9O4H2
R361C5H9O4H2
R362C5H9O4H2
R363C5H9O4H2
R364C5H9O4H2
R365C5H10OOOOH
R366C4H8OOOOH
R367C5H9O4H2
R368C3H5O4H2
R369C4H7O4H2
R370C5H9O4H2

R371C5H9O4H2
R372C7H13O4H2
R373C7H13O4H2
R374C5H9O4H2
R375C7H13O4H2
R376C3H5O4H2
R377C4H7O4H2
R378C7H13O4H2
R379C7H13O4H2
R380C7H13O4H2
R381C7H13O4H2
R382C4H8OOOOH
R383C5H9OO4H2
R384C4H7O4H2
R385C5H9OO4H2
R386C4H7OHOOOOH
R387C6H11OO4H2
R388C4H7OO4H2
R389C6H11OO4H2
R390C5H9O4H2
R391C5H9O4H2
R392C5H9O4H2
R393C4H7O4H2
R394C4H8OOOOH
R395C5H10OOOOH
R396C5H9O4H2
R397C3H6OOOOH
R398C4H7O4H2
R399C4H7O4H2
R400C4H8OOOOH
R401C4H6OHO4H2
R402C4H6OHO4H2
R403C4H7OHOOOOH
R404C4H7O4H2
R405C4H8OOH
R406C5H10OOH
R407C3H6OOH
R408C4H7O4H2
R409C4H8OOH
R410C4H6OHO4H2
R411C4H7OHOOH
R1C5H11O
R2C5H11O
R1C4H9O
R2C4H9O
RC6H13

! lumped Free radicals :
.C3H5Y
.C4H7Y
.COC2H5
.C5H9Y
.COC3H7
.COC4H9
.COC6H13
.COC5H11
.COOC3H7
.COOC2H5
.COOOC2H5
.COOOC3H7
.COOOC4H9
.COOOC6H13
.COOOC5H11

```
! lumped Cyclic free radicals :
.C3H5O#4
.C4H7O#4
.C4H7O#5
.C7H13O#4
.C7H13O#5
.C7H13O#6
.C5H9O#4
.C5H9O#5
.C5H9O#6
.OOC3H5O#4
.OOC4H7O#4
.OOC4H7O#5
.OOC7H13O#4
.OOC7H13O#5
.OOC7H13O#6
.OOC5H9O#4
.OOC5H9O#5
.OOC5H9O#6
.C3H4O#4OOH
.C4H6O#4OOH
.C4H6O#5OOH
.C7H12O#4OOH
.C7H12O#5OOH
.C7H12O#6OOH
.C5H8O#4OOH
.C5H8O#5OOH
.C5H8O#6OOH
.OOC3H4O#4OOH
.OOC4H6O#4OOH
.OOC4H6O#5OOH
.OOC7H12O#4OOH
.OOC7H12O#5OOH
.OOC7H12O#6OOH
.OOC5H8O#4OOH
.OOC5H8O#5OOH
.OOC5H8O#6OOH

N2
HE
END

THERMO ALL
   300.000  1000.000  5000.000
R1C5H11O                C   5H  11O   1     G  0300.00   5000.00  1000.00      1
 1.55470E+01    2.41453E-02   -6.84426E-06    9.51344E-10   -5.28979E-14       2
-2.18664E+04   -5.16209E+01   -2.40073E+00    8.04985E-02   -7.81085E-05       3
 4.40257E-08   -1.02639E-11   -1.70670E+04    3.98312E+01                      4
R2C5H11O                C   5H  11O   1     G  0300.00   5000.00  1000.00      1
 1.69994E+01    2.29874E-02   -6.45552E-06    8.88452E-10   -4.89064E-14       2
-2.22790E+04   -6.26895E+01   -2.15523E+00    8.13023E-02   -7.73437E-05       3
 4.23708E-08   -9.82108E-12   -1.70686E+04    3.53707E+01                      4
RC6H13                  C   6H  13O   0     G  0300.00   5000.00  1000.00      1
 1.09570E+01    3.73235E-02   -1.21518E-05    1.86634E-09   -1.11273E-13       2
-1.41053E+03   -2.61478E+01   -4.37655E-01    7.11136E-02   -4.36744E-05       3
 9.68595E-09    1.20258E-12    1.37897E+03    3.16000E+01                      4
R1C4H9O                 C   4H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R2C4H9O                 C   4H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
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```
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                   C   1H   2O   1      G  0300.00   5000.00  1000.00      1
 2.91430E+00    6.64407E-03   -2.45282E-06    4.12836E-10   -2.63040E-14       2
-1.52827E+04    7.43680E+00    2.41049E+00    7.02041E-03   -4.22947E-06       3
 4.40116E-09   -2.12647E-12   -1.49519E+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
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CH3O2H                  C   1H   4O   2     G  0300.00   5000.00  1000.00      1
 6.37596E+00    1.07372E-02   -3.68666E-06    5.88827E-10   -3.61266E-14       2
-1.84341E+04   -6.12840E+00    3.09218E+00    1.80223E-02   -7.11862E-06       3
-1.47978E-09    1.45517E-12   -1.74300E+04    1.13028E+01                      4
C2H2                    C   2H   2O   0     G  0300.00   5000.00  1000.00      1
 3.00338E+00    7.58476E-03   -3.11008E-06    5.64312E-10   -3.79570E-14       2
 2.62468E+04    5.29247E+00    2.54593E+00    1.14007E-02   -7.07123E-06       3
-6.00363E-10    1.71894E-12    2.60564E+04    6.56609E+00                      4
C2H4Z                   C   2H   4O   0     G  0300.00   5000.00  1000.00      1
 3.99720E-01    1.67299E-02   -6.80909E-06    1.22922E-09   -8.23928E-14       2
 5.63749E+03    1.97729E+01    1.31810E+00    1.44460E-02   -2.74335E-06       3
-3.10835E-09    1.52772E-12    5.26817E+03    1.47233E+01                      4
C2H6                    C   2H   6O   0     G  0300.00   5000.00  1000.00      1
 3.94109E-01    2.11928E-02   -8.08560E-06    1.39339E-09   -9.03005E-14       2
-1.10714E+04    1.96366E+01    9.75454E-01    1.88110E-02   -1.46453E-06       3
-6.38247E-09    2.84067E-12   -1.13111E+04    1.65514E+01                      4
CH2COZ                  C   2H   2O   1     G  0300.00   5000.00  1000.00      1
 5.35267E+00    6.94209E-03   -2.50061E-06    4.13231E-10   -2.59692E-14       2
-7.81007E+03   -3.80283E+00    2.99539E+00    1.23540E-02   -4.06499E-06       3
-3.34608E-09    2.24152E-12   -7.15097E+03    8.53716E+00                      4
CH3CHO                 0C   2H   4O   1     G  0300.00   5000.00  1000.00      1
 0.05869E+02    0.10794E-01   -0.03646E-04    0.05413E-08   -0.02897E-12       2
-0.02265E+06   -0.06013E+02   -5.97842E+01    4.89059E-01   -1.27143E-03       3
 1.42135E-06   -5.67547E-10   -1.52478E+04    2.71669E+02                      4
 !coefficients de CHEMKIN a haute temperature et THERGAS a basse temperature!
C2H5OH                  C   2H   6O   1     G  0300.00   5000.00  1000.00      1
 5.62516E+00    1.59916E-02   -5.36799E-06    8.43422E-10   -5.11406E-14       2
-3.10498E+04   -3.61961E+00    9.39858E-01    2.61811E-02   -9.25134E-06       3
-3.45825E-09    2.62098E-12   -2.96238E+04    2.12634E+01                      4
C2H5O2H                 C   2H   6O   2     G  0300.00   5000.00  1000.00      1
 8.86549E+00    1.46991E-02   -4.66630E-06    7.03129E-10   -4.13262E-14       2
-2.34663E+04   -1.74646E+01    2.03266E+00    3.20310E-02   -1.79773E-05       3
 2.38766E-09    1.07206E-12   -2.15063E+04    1.82187E+01                      4
CH3COO2H                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
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                   0C   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
C4H6Z2                 0C   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
C4H8Y                  0C   4H   8          G  0300.00   5000.00  1000.00      1
 .12072002E+02  .17483519E-01  -.47358262E-05 .63614963E-09 -.34500855E-13       2
 .34200605E+04 -.37559532E+02  -.86302972E+00 .53421453E-01 -.45552202E-04       3
 .24475971E-07 -.60568863E-11   .72361128E+04 .29821739E+02                      4
C4H10                  0C   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
C2H3CHO                0C   3H   4O   1     G  0300.00   5000.00  1000.00      1
  .12311886E+02  .12961588E-01 -.61774654E-05  .12501405E-08 -.91169971E-13       2
 -.15218951E+05 -.42303177E+02  .93137437E+00  .35574418E-01 -.33347264E-04       3
  .28398034E-07 -.11395644E-10 -.10614329E+05  .21059492E+02                      4
C2H5CHO                0C   3H   6O   1     G  0300.00   5000.00  1000.00      1
  .70107722E+01  .18013448E-01 -.62295217E-05  .10005839E-08 -.61661722E-13       2
 -.25691457E+05 -.95488281E+01  .28277023E+01  .25430365E-01 -.61913220E-05       3
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 -.50245177E-08  .26785609E-11 -.24271348E+05  .13234089E+02                   4
C3H7OH                  0C   3H   8O   1     G  0300.00   5000.00  1000.00     1
  .71674681E+01  .22466624E-01 -.76292372E-05  .12097231E-08 -.73884075E-13    2
 -.34686773E+05 -.95393562E+01  .12350693E+01  .34453284E-01 -.10589133E-04    3
 -.54856804E-08  .35146994E-11 -.32804938E+05  .22268148E+02                   4
C2H6CO                  0C   3H   6O   1     G  0300.00   5000.00  1000.00     1
  .59975996E+01  .19679097E-01 -.70154574E-05  .11513579E-08 -.72035416E-13    2
 -.29362656E+05 -.55254784E+01  .14577827E+01  .28063715E-01 -.90218518E-05    3
 -.24536706E-08  .16730232E-11 -.27794104E+05  .19218454E+02                   4
C3H8CO                  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
R1H                     C   0H   1O   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   1O   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
 3.90412E+03    4.81762E+00    3.67780E+00   -2.14153E-04    5.70231E-08      3
 1.71404E-10   -1.84629E-14    3.63597E+03    1.19670E+00                    4
R3O2H                   C   0H   1O   2     G  0300.00   5000.00  1000.00     1
 4.72022E+00    1.38622E-03   -1.68457E-07    1.05843E-11   -2.40717E-16      2
-2.41430E+02   -6.85165E-01    1.84854E+00    1.07988E-02   -8.54635E-06      3
 4.18415E-10    1.44074E-12    3.26446E+02    1.34319E+01                    4
R4CH3                   C   1H   3O   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   1O   1     G  0300.00   5000.00  1000.00     1
 4.39893E+00    1.53560E-03   -1.99211E-07    1.43007E-11   -4.51357E-16      2
 1.46590E+03    1.23461E+00    2.96884E+00    5.16190E-03   -6.79642E-06      3
 7.15025E-09   -2.73201E-12    2.04422E+03    9.08982E+00                    4
R6CH2OH                 C   1H   3O   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   3O   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   3O   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   1O   0     G  0300.00   5000.00  1000.00     1
 6.02264E+00    8.77475E-04   -8.67941E-08    3.67081E-12    1.93550E-17      2
 6.20557E+04   -9.36163E+00    1.89603E+00    1.61116E-02   -1.74770E-05      3
 5.93645E-09    3.50654E-13    6.28086E+04    1.05397E+01                    4
R10C2H3V                C   2H   3O   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   5O   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   1O   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               C   2H   3O   1     G  0300.00   5000.00  1000.00     1
 0.05976E+02    0.08131E-01   -0.02744E-04    0.04070E-08   -0.02176E-12      2
 0.04903E+04   -0.05045E+02   -5.49040E+01    4.51253E-01   -1.17037E-03      3
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 1.30375E-06   -5.19201E-10    7.54530E+03    2.51103E+02                    4
 !coefficients de CHEMKIN a haute temperature et THERGAS a basse temperature!
R14CH3CO               C   2H   3O   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   5O   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
R16C2H4O2H             C   2H   5O   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   5O   2     G  0300.00   5000.00  1000.00      1
 1.13253E+01    8.28625E-03   -1.86203E-06    2.18209E-10   -1.07868E-14       2
-6.98659E+03   -3.29488E+01    6.72056E-01    3.62757E-02   -3.00008E-05       3
 1.38479E-08   -2.84583E-12   -3.78886E+03    2.28869E+01                    4
R18CH3COOO             C   2H   3O   3     G  0300.00   5000.00  1000.00      1
 1.10774E+01    6.59595E-03   -1.40685E-06    1.55610E-10   -7.22472E-15       2
-1.93998E+04   -2.93379E+01   -1.25738E+00    4.04124E-02   -3.66489E-05       3
 1.70556E-08   -3.15366E-12   -1.58216E+04    3.48253E+01                    4
R19C3H7                C   3H   7O   0     G  0300.00   5000.00  1000.00      1
 4.90850E+00    1.95492E-02   -6.09862E-06    9.08986E-10   -5.30994E-14       2
 9.72711E+03    2.41566E-01   -9.97049E-01    4.22637E-02   -3.67683E-05       3
 1.83985E-08   -3.66617E-12    1.08489E+04    2.87294E+01                    4
R20C4H9                C   4H   9O   0     G  0300.00   5000.00  1000.00      1
 7.04485E+00    2.53221E-02   -8.04531E-06    1.21383E-09   -7.14512E-14       2
 5.52642E+03   -9.13080E+00   -5.06119E-01    5.07221E-02   -3.74398E-05       3
 1.45966E-08   -1.90079E-12    7.19571E+03    2.83231E+01                    4
C7H16                  C   7H  16O   0     G  0300.00   5000.00  1000.00      1
 1.35144E+01    4.73250E-02   -1.67455E-05    2.73490E-09   -1.70591E-13       2
-3.16323E+04   -4.69225E+01   -1.99469E+00    8.37785E-02   -3.04588E-05       3
-1.67886E-08    1.21089E-11   -2.73539E+04    3.40515E+01                    4
C5H12O                 C   5H  12O   1     G  0300.00   5000.00  1000.00      1
 1.26405E+01    3.32576E-02   -1.13614E-05    1.80776E-09   -1.10601E-13       2
-4.10682E+04   -4.07635E+01   -1.08794E+00    7.07602E-02   -4.51849E-05       3
 1.09959E-08    7.10346E-13   -3.72778E+04    3.02105E+01                    4
C6H14O                 C   6H  14O   1     G  0300.00   5000.00  1000.00      1
 1.38213E+01    4.01951E-02   -1.38177E-05    2.20876E-09   -1.35592E-13       2
-4.56940E+04   -4.44699E+01    4.32642E+00    4.11295E-02    4.96243E-05       3
-8.84877E-08    3.57521E-11   -4.23171E+04    9.72322E+00                    4
C5H10Z                 C   5H  10O   0     G  0300.00   5000.00  1000.00      1
 6.80754E+00    3.28105E-02   -1.18208E-05    1.95584E-09   -1.23143E-13       2
-7.71758E+03   -8.25185E+00    8.75607E-01    4.50825E-02   -1.19396E-05       3
-1.06759E-08    6.26846E-12   -6.00243E+03    2.31246E+01                    4
C6H12Z                 C   6H  12O   0     G  0300.00   5000.00  1000.00      1
 9.34166E+00    3.83481E-02   -1.37169E-05    2.25582E-09   -1.41304E-13       2
-1.00855E+04   -1.92090E+01    2.53267E-01    5.81443E-02   -1.64643E-05       3
-1.50795E-08    9.21032E-12   -7.51592E+03    2.85895E+01                    4
C4H8OY                 C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 8.51493E+00    2.46786E-02   -8.59220E-06    1.38637E-09   -8.56917E-14       2
-2.14037E+04   -1.61753E+01    2.83583E+00    3.50566E-02   -9.00815E-06       3
-6.74033E-09    3.74329E-12   -1.95091E+04    1.46363E+01                    4
C5H10OY                C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.06775E+01    3.03637E-02   -1.05164E-05    1.69145E-09   -1.04364E-13       2
-2.65713E+04   -2.56642E+01    1.02499E+00    5.42710E-02   -2.73447E-05       3
 1.48991E-09    2.63937E-12   -2.37614E+04    2.49009E+01                    4
C3H5OOHY               C   3H   6O   2     G  0300.00   5000.00  1000.00      1
 2.00143E+01    2.60796E-03    1.40085E-06   -5.76414E-10    5.53922E-14       2
-2.13224E+04   -8.52498E+01    1.76581E+00    3.44145E-02   -1.14827E-05       3
-1.68197E-09    5.92817E-13   -1.45137E+04    1.56758E+01                    4
C6H11OOHZ              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 3.67351E+01    2.76270E-03    3.70050E-06   -1.26841E-09    1.15437E-13       2
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-3.58248E+04   -1.71040E+02    2.66378E+00    6.18677E-02   -1.91101E-05       3
-4.92051E-09    1.74249E-12   -2.31149E+04    1.74269E+01                      4
C7H14Z                 C   7H  14O   0     G  0300.00   5000.00  1000.00      1
 1.13867E+01    4.42145E-02   -1.57120E-05    2.57149E-09   -1.60503E-13       2
-1.36130E+04   -2.81944E+01    2.04441E-01    6.90021E-02   -2.12527E-05       3
-1.58288E-08    1.01515E-11   -1.04399E+04    3.05884E+01                      4
C4H7OOHY               C   4H   8O   2     G  0300.00   5000.00  1000.00      1
 2.46072E+01    3.38408E-03    2.09012E-06   -8.29222E-10    7.89031E-14       2
-2.70846E+04   -1.08199E+02    4.65242E-01    4.55966E-02   -1.53359E-05       3
-1.92597E-09    6.80415E-13   -1.80863E+04    2.52831E+01                      4
C5H9OOHZ               C   5H  10O   2     G  0300.00   5000.00  1000.00      1
 3.09781E+01    2.95561E-03    2.89772E-06   -1.04345E-09    9.65032E-14       2
-3.08257E+04   -1.41161E+02    2.25982E+00    5.36444E-02   -1.91077E-05       3
-1.14560E-09    4.07159E-13   -2.01533E+04    1.74886E+01                      4
C4H7OOOHY              C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 2.40573E+01    7.11428E-03    1.05393E-06   -7.40497E-10    7.89644E-14       2
-4.17629E+04   -1.01819E+02    2.69167E+00    4.43417E-02   -1.46885E-05       3
-9.26927E-10    3.28052E-13   -3.37667E+04    1.64130E+01                      4
C5H9OOOHY              C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 2.96044E+01    7.12694E-03    1.94690E-06   -1.01154E-09    1.02576E-13       2
-4.77877E+04   -1.30692E+02    3.05700E+00    5.40169E-02   -1.92361E-05       3
 2.35665E-10   -8.47165E-14   -3.78987E+04    1.60231E+01                      4
C6H12OZ                C   6H  12O   1     G  0300.00   5000.00  1000.00      1
 1.36623E+01    3.54188E-02   -1.22429E-05    1.96716E-09   -1.21334E-13       2
-3.31135E+04   -4.30323E+01   -1.19413E+00    7.73859E-02   -5.21059E-05       3
 1.43428E-08    2.14923E-13   -2.91141E+04    3.33477E+01                      4
C3H7CHO                C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 8.11156E+00    2.54239E-02   -8.96011E-06    1.45917E-09   -9.08294E-14       2
-2.99254E+04   -1.52603E+01   -1.14394E+00    4.85922E-02   -2.49936E-05       3
 4.93978E-10    2.97345E-12   -2.72812E+04    3.30785E+01                      4
C6H14CO                C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 1.46417E+01    4.22620E-02   -1.45836E-05    2.33774E-09   -1.43806E-13       2
-4.34356E+04   -4.31866E+01    2.13601E+00    6.91818E-02   -2.49511E-05       3
-8.53288E-09    6.65016E-12   -3.95751E+04    2.33889E+01                      4
C4H9CHO                C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.06444E+01    3.07316E-02   -1.07309E-05    1.73589E-09   -1.07536E-13       2
-3.46381E+04   -2.91755E+01   -1.74961E+00    6.25390E-02   -3.39263E-05       3
 1.68936E-09    3.69646E-12   -3.11651E+04    3.52944E+01                      4
C6H13CHO               C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 1.52350E+01    4.14563E-02   -1.42334E-05    2.27397E-09   -1.39584E-13       2
-3.98300E+04   -4.57640E+01    2.50111E+00    6.97502E-02   -2.73800E-05       3
-6.13701E-09    5.83515E-12   -3.59532E+04    2.17877E+01                      4
C4H9OCHO               C   5H  10O   2     G  0300.00   5000.00  1000.00      1
 1.40534E+01    2.98067E-02   -1.02534E-05    1.63952E-09   -1.00653E-13       2
-6.29179E+04   -4.46016E+01   -2.62991E+00    8.11729E-02   -6.55756E-05       3
 2.41363E-08   -2.00404E-12   -5.87205E+04    3.99142E+01                      4
C5H11OCHO              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 3.67774E+01    1.04721E-03    4.26136E-06   -1.32443E-09    1.16487E-13       2
-6.46141E+04   -1.70866E+02    4.31544E+00    5.82329E-02   -1.99191E-05       3
-2.42617E-09    8.63463E-13   -5.25588E+04    8.45817E+00                      4
C2H5COOOH              C   3H   6O   3     G  0300.00   5000.00  1000.00      1
 1.04998E+01    1.90673E-02   -6.32815E-06    9.87705E-10   -5.96899E-14       2
-4.77560E+04   -2.15710E+01    6.24713E-02    5.05444E-02   -3.96557E-05       3
 1.45425E-08   -1.34983E-12   -4.50787E+04    3.15183E+01                      4
C5H12OCO               C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 1.61641E+01    3.51720E-02   -1.19656E-05    1.89749E-09   -1.15773E-13       2
-7.05382E+04   -5.45155E+01   -3.45805E+00    9.54112E-02   -7.61716E-05       3
 2.72582E-08   -1.93721E-12   -6.56095E+04    4.48953E+01                      4
C2H4CHOOOH             C   3H   6O   3     G  0300.00   5000.00  1000.00      1
 1.24388E+01    1.64061E-02   -5.17148E-06    7.75411E-10   -4.54214E-14       2
-3.69015E+04   -3.03517E+01    4.94995E+00    3.35249E-02   -1.43099E-05       3
-2.56567E-09    2.79709E-12   -3.46591E+04    9.23311E+00                      4
C3H6CHOOOH             C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 1.34614E+01    2.39058E-02   -7.91389E-06    1.23217E-09   -7.42907E-14       2
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-4.10977E+04   -3.49129E+01    1.05406E+00    5.61509E-02   -3.17949E-05       3
 1.60319E-09    3.58336E-12   -3.76769E+04    2.94511E+01                      4
C6H13COOOH             C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 1.88013E+01    4.23677E-02   -1.42446E-05    2.23998E-09   -1.35862E-13       2
-6.19255E+04   -5.82166E+01    9.99067E-02    9.23433E-02   -5.47989E-05       3
 7.40686E-09    3.93464E-12   -5.67996E+04    3.85298E+01                      4
C6H12CHOOOH            C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 2.06226E+01    3.98945E-02   -1.31806E-05    2.04777E-09   -1.23198E-13       2
-5.10208E+04   -6.63311E+01    4.84381E+00    7.63010E-02   -3.17526E-05       3
-7.45549E-09    7.30401E-12   -4.63643E+04    1.68551E+01                      4
C4H8OCHOOOH            C   5H  10O   4     G  0300.00   5000.00  1000.00      1
 1.94928E+01    2.81592E-02   -9.15571E-06    1.40330E-09   -8.34627E-14       2
-7.41300E+04   -6.43613E+01   -4.62869E-01    8.89495E-02   -7.29121E-05       3
 2.57956E-08   -1.59578E-12   -6.91130E+04    3.68231E+01                      4
C5H10OCHOOOH           C   6H  12O   4     G  0300.00   5000.00  1000.00      1
 4.17107E+01    2.52991E-03    4.04156E-06   -1.35675E-09    1.22666E-13       2
-8.07610E+04   -1.96280E+02    4.46697E+00    6.82090E-02   -2.41362E-05       3
-1.99100E-09    7.07966E-13   -6.69228E+04    9.46535E+00                      4
C5H11OCOOOH            C   6H  12O   4     G  0300.00   5000.00  1000.00      1
 3.76594E+01    4.96227E-04    5.42431E-06   -1.62731E-09    1.41196E-13       2
-1.14745E+05   -1.80266E+02    2.75420E+00    6.13283E-02   -1.84438E-05       3
-5.14337E-09    1.82117E-12   -1.01757E+05    1.27048E+01                      4
C3H7COOOH              C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H8CHOOOH             C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 1.65202E+01    2.81645E-02   -9.18066E-06    1.41233E-09   -8.43649E-14       2
-4.39563E+04   -4.82809E+01    4.76538E+00    5.58247E-02   -2.52183E-05       3
-2.83332E-09    4.28260E-12   -4.04977E+04    1.36010E+01                      4
C4H9COOOH              C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H10CO                C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.02079E+01    3.10176E-02   -1.07948E-05    1.74025E-09   -1.07443E-13       2
-3.64743E+04   -2.47274E+01   -2.91355E-01    5.41823E-02   -2.07811E-05       3
-6.39126E-09    5.32339E-12   -3.32819E+04    3.09801E+01                      4
C2H4COO4H2             C   3H   6O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C3H4OHOOHZ             C   3H   6O   3     G  0300.00   5000.00  1000.00      1
 2.16516E+01    2.42885E-03    1.82119E-06   -6.92078E-10    6.50855E-14       2
-4.25733E+04   -8.85603E+01    1.32293E+00    3.85207E-02   -1.44784E-05       3
 4.41570E-11   -1.43138E-14   -3.50255E+04    2.36975E+01                      4
C3H5OHY                C   3H   6O   1     G  0300.00   5000.00  1000.00      1
 1.78424E+01    5.68413E-05    2.10571E-06   -6.22135E-10    5.36614E-14       2
-2.66552E+04   -6.98571E+01    2.59658E+00    2.75242E-02   -1.10673E-05       3
 7.25320E-10   -2.55190E-13   -2.10272E+04    1.42043E+01                      4
C4H9OCOOOH             C   5H  10O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H6O4H2Y              C   4H   8O   4     G  0300.00   5000.00  1000.00      1
 3.09377E+01    3.82086E-03    1.80778E-06   -7.71964E-10    7.49165E-14       2
-4.15843E+04   -1.42789E+02    1.67842E+00    5.43180E-02   -1.72842E-05       3
-4.17476E-09    1.47506E-12   -3.06389E+04    1.91604E+01                      4
C3H5OHCHOOOH           C   4H   8O   4     G  0300.00   5000.00  1000.00      1
 3.31723E+01   -5.42636E-04    2.58835E-06   -7.18963E-10    6.05243E-14       2
-7.48881E+04   -1.50789E+02    2.28824E+00    5.46606E-02   -2.27398E-05       3
 6.92253E-10   -2.45499E-13   -6.34546E+04    1.96171E+01                      4
C3H6OHCHO              C   4H   8O   2     G  0300.00   5000.00  1000.00      1
 2.77403E+01   -9.83918E-04    2.15619E-06   -5.60610E-10    4.60781E-14       2
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-5.85761E+04   -1.22687E+02    2.28795E+00    4.36327E-02   -1.59902E-05       3
-2.27522E-09    8.07235E-13   -4.91068E+04    1.79700E+01                      4
C4H9OH                C   4H  10O   1     G  0300.00   5000.00  1000.00      1
 9.74596E+00    2.77326E-02   -9.38444E-06    1.48350E-09   -9.03664E-14       2
-3.91909E+04   -2.34734E+01    1.11535E-02    5.09795E-02   -2.33511E-05       3
-1.86774E-09    3.69534E-12   -3.63433E+04    2.76793E+01                      4
C4H9OOH               C   4H  10O   2     G  0300.00   5000.00  1000.00      1
 1.31827E+01    2.62065E-02   -8.57668E-06    1.32258E-09   -7.91032E-14       2
-3.16741E+04   -3.81353E+01    1.47066E+00    5.47675E-02   -2.64877E-05       3
-2.05538E-09    4.34286E-12   -2.83122E+04    2.31835E+01                      4
C3H7OOH               C   3H   8O   2     G  0300.00   5000.00  1000.00      1
 1.08540E+01    2.06660E-02   -6.72020E-06    1.03292E-09   -6.17108E-14       2
-2.69712E+04   -2.61346E+01    2.01919E+00    4.26576E-02   -2.22417E-05       3
 1.14166E-09    2.18158E-12   -2.44343E+04    2.00658E+01                      4
C5H12                 C   5H  12O   0     G  0300.00   5000.00  1000.00      1
 5.76039E+00    4.07904E-02   -1.51216E-05    2.55218E-09   -1.62906E-13       2
-2.23578E+04   -3.87465E+00   -2.51012E-01    5.37447E-02   -1.29532E-05       3
-1.58241E-08    9.07402E-12   -2.07997E+04    2.74284E+01                      4
C5H11OH               C   5H  12O   1     G  0300.00   5000.00  1000.00      1
 1.06951E+01    3.58706E-02   -1.25170E-05    2.02384E-09   -1.25331E-13       2
-4.11002E+04   -3.12983E+01   -1.75632E+00    6.39598E-02   -2.59868E-05       3
-6.14445E-09    5.85383E-12   -3.73572E+04    3.45867E+01                      4
C4H10O                C   4H  10O   1     G  0300.00   5000.00  1000.00      1
 1.01807E+01    2.77890E-02   -9.51259E-06    1.51652E-09   -9.29478E-14       2
-3.53741E+04   -2.64667E+01   -7.61343E-01    5.76814E-02   -3.68938E-05       3
 9.63579E-09    1.86539E-13   -3.23368E+04    3.01404E+01                      4
C6H14                 C   6H  14O   0     G  0300.00   5000.00  1000.00      1
 1.00922E+01    4.25999E-02   -1.51299E-05    2.47781E-09   -1.54864E-13       2
-2.70709E+04   -2.76053E+01   -1.08806E+00    6.84694E-02   -2.44048E-05       3
-1.16936E-08    8.57931E-12   -2.39377E+04    3.09333E+01                      4
C8H18                 C   8H  18O   0     G  0300.00   5000.00  1000.00      1
 1.69837E+01    5.19663E-02   -1.83122E-05    2.98040E-09   -1.85358E-13       2
-3.62133E+04   -6.78903E+01   -2.59900E+00    9.70062E-02   -3.15501E-05       3
-2.68048E-08    1.73705E-11   -3.08027E+04    3.45010E+01                      4
C7H15OOH              C   7H  16O   2     G  0300.00   5000.00  1000.00      1
 1.90583E+01    4.41095E-02   -1.47049E-05    2.29930E-09   -1.38956E-13       2
-4.10938E+04   -6.22202E+01    2.08463E+00    8.42854E-02   -3.70758E-05       3
-6.15297E-09    7.46171E-12   -3.61582E+04    2.69564E+01                      4
C5H11OOOH             C   5H  12O   3     G  0300.00   5000.00  1000.00      1
 1.81982E+01    3.04318E-02   -9.64979E-06    1.45660E-09   -8.59203E-14       2
-5.68418E+04   -6.31782E+01   -2.16010E+00    8.68509E-02   -5.52385E-05       3
 4.78684E-09    6.09585E-12   -5.15658E+04    4.11716E+01                      4
C6H13OOOH             C   6H  14O   3     G  0300.00   5000.00  1000.00      1
 1.92078E+01    3.86471E-02   -1.27812E-05    1.98778E-09   -1.19711E-13       2
-5.68865E+04   -6.57284E+01    6.18745E+00    5.10129E-02    3.72900E-05       3
-8.19279E-08    3.44611E-11   -5.26767E+04    6.13805E+00                      4
C5H11OOH              C   5H  12O   2     G  0300.00   5000.00  1000.00      1
 1.50370E+01    3.24970E-02   -1.07846E-05    1.68024E-09   -1.01251E-13       2
-3.60103E+04   -4.53778E+01    6.31097E+00    3.50610E-02    4.04087E-05       3
-7.25720E-08    2.91810E-11   -3.29241E+04    4.16890E+00                      4
C4H8OHOOH             C   4H  10O   3     G  0300.00   5000.00  1000.00      1
 1.54458E+01    2.61300E-02   -8.40633E-06    1.28287E-09   -7.62956E-14       2
-5.36659E+04   -4.77450E+01    5.52607E+00    3.89805E-02    1.75303E-05       3
-4.86827E-08    2.10700E-11   -5.05548E+04    6.32798E+00                      4
C4H7OHY               C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H6YZ                C   4H   6O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C5H9OHZ               C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C5H8Z2                 C   5H   8O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C5H11CHO               C   6H  12O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11OHZ               C   6H  12O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H10Z2                C   6H  10O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C3H7COOH               C   4H   8O   2     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C2H5COOH               C   3H   6O   2     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C3H5CHOY               C   4H   6O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H10Y2                C   6H  10O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C7H12Y2                C   7H  12O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C8H14Y2                C   8H  14O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H7CHOY               C   5H   8O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C9H16Y2                C   9H  16O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C5H9CHOY               C   6H  10O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C10H18Y2               C  10H  18O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C2H4O#3                C   2H   4O   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   -1.34620E+00   -9.24908E-01    2.64513E-02   -1.34725E-05       3
 3.74058E-10    1.40310E-12   -7.13279E+03    2.71327E+01                      4
C3H6O#3                C   3H   6O   1     G  0300.00   5000.00  1000.00      1
 7.29482E+00    1.84105E-02   -6.54108E-06    1.07188E-09   -6.70432E-14       2
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-1.50956E+04   -1.44063E+01    9.39739E-02    3.50454E-02   -2.55405E-05       3
 1.69102E-08   -6.38433E-12   -1.25752E+04    2.45001E+01                      4
C3H6O#4                C   3H   6O   1     G  0300.00   5000.00  1000.00      1
-2.80859E-01    3.28683E-02   -1.41730E-05    2.66755E-09   -1.84356E-13       2
-1.13051E+04    2.38104E+01    1.54114E+00    1.02641E-02    4.43080E-05       3
-5.54504E-08    2.02306E-11   -1.08722E+04    1.88571E+01                      4
C4H8O#3                C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 1.05870E+01    2.25034E-02   -7.73286E-06    1.23527E-09   -7.57683E-14       2
-2.07171E+04   -3.27019E+01   -4.21162E-01    4.56121E-02   -1.34695E-05       3
-1.27714E-08    7.56466E-12   -1.73775E+04    2.58582E+01                      4
C4H8O#4                C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 1.29825E+00    3.95230E-02   -1.64598E-05    3.02134E-09   -2.05012E-13       2
-1.56877E+04    1.67608E+01    1.11342E+00    2.14875E-02    4.23549E-05       3
-6.11470E-08    2.33673E-11   -1.47625E+04    2.21621E+01                      4
C4H8O#5                C   4H   8O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
-2.21935E+04    1.81160E+01    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00   -2.21935E+04    1.81160E+01                      4
C7H14O#3               C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 1.54763E+01    4.15117E-02   -1.43184E-05    2.29499E-09   -1.41190E-13       2
-2.86862E+04   -5.02284E+01    4.15455E+00    4.58073E-02    4.31824E-05       3
-7.96415E-08    3.13801E-11   -2.44994E+04    1.43652E+01                      4
C7H14O#4               C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 9.15757E+00    5.53005E-02   -2.15324E-05    3.76620E-09   -2.46754E-13       2
-3.01327E+04   -2.12215E+01   -8.73323E+00    1.22435E-01   -1.25044E-04       3
 7.71721E-08   -1.95490E-11   -2.57960E+04    6.73425E+01                      4
C7H14O#5               C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 1.78766E+01    4.05575E-02   -1.42848E-05    2.32527E-09   -1.44695E-13       2
-4.21610E+04   -6.80840E+01   -4.33123E+00    1.08064E-01   -8.76521E-05       3
 3.40106E-08   -3.83186E-12   -3.64344E+04    4.48596E+01                      4
C7H14O#6               C   7H  14O   1     G  0300.00   5000.00  1000.00      1
 1.79352E+01    4.04535E-02   -1.42239E-05    2.31091E-09   -1.43518E-13       2
-4.49021E+04   -7.11286E+01   -4.34214E+00    1.08133E-01   -8.78054E-05       3
 3.41502E-08   -3.87705E-12   -3.91506E+04    4.21892E+01                      4
C5H10O2#4              C   5H  10O   2     G  0300.00   5000.00  1000.00      1
 1.55088E+01    2.82516E-02   -9.64408E-06    1.53448E-09   -9.39221E-14       2
-5.31419E+04   -5.93589E+01   -6.80362E+00    9.78303E-02   -8.45064E-05       3
 3.11668E-08   -2.17586E-12   -4.76564E+04    5.32656E+01                      4
C6H12O2#4              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 1.80532E+01    3.35437E-02   -1.14099E-05    1.81052E-09   -1.10588E-13       2
-5.95210E+04   -7.15001E+01   -7.24418E+00    1.10568E-01   -9.04293E-05       3
 2.92853E-08   -3.45794E-13   -5.32175E+04    5.66345E+01                      4
C6H12O2#5              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 1.75422E+01    3.52108E-02   -1.23017E-05    1.99002E-09   -1.23240E-13       2
-5.56154E+04   -7.03827E+01   -5.33872E+00    1.08477E-01   -9.95233E-05       3
 4.66783E-08   -8.05763E-12   -4.98789E+04    4.51049E+01                      4
C6H12O2#3              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 1.69472E+01    3.30855E-02   -1.09038E-05    1.68994E-09   -1.01438E-13       2
-4.82397E+04   -6.19885E+01   -3.41320E+00    8.02228E-02   -2.94632E-05       3
-2.09503E-08    1.43264E-11   -4.24870E+04    4.47384E+01                      4
C5H10O#3               C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.26360E+01    2.83756E-02   -9.74015E-06    1.55503E-09   -9.53599E-14       2
-2.42489E+04   -4.03304E+01   -3.23154E-01    5.54559E-02   -1.58231E-05       3
-1.59623E-08    9.37634E-12   -2.03173E+04    2.86205E+01                      4
C5H10O#4               C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 5.50836E+00    4.29493E-02   -1.73432E-05    3.11330E-09   -2.07830E-13       2
-2.32692E+04   -5.76836E+00   -8.90000E+00    1.02609E-01   -1.20193E-04       3
 8.36221E-08   -2.32794E-11   -1.99203E+04    6.44578E+01                      4
C5H10O#5               C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.30482E+01    2.95132E-02   -1.05347E-05    1.73093E-09   -1.08410E-13       2
-3.27552E+04   -4.50173E+01   -3.27847E+00    7.95042E-02   -6.64727E-05       3
 2.78256E-08   -3.98393E-12   -2.85265E+04    3.80121E+01                      4
C5H10O#6               C   5H  10O   1     G  0300.00   5000.00  1000.00      1
 1.17730E+01    3.09452E-02   -1.11277E-05    1.83880E-09   -1.15674E-13       2
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-3.28419E+04   -4.02061E+01    1.42171E+00    4.72724E-02    4.18457E-06       3
-3.64031E-08    1.68516E-11   -2.95912E+04    1.58204E+01                      4
C3H5O#3OOH             C   3H   6O   3     G  0300.00   5000.00  1000.00      1
 1.04805E+01    2.06196E-02   -7.24496E-06    1.17707E-09   -7.31324E-14       2
-3.19832E+04   -2.65595E+01   -1.13006E+00    4.98703E-02   -2.41021E-05       3
-6.43910E-09    6.75663E-12   -2.88409E+04    3.36527E+01                      4
C3H5O#4OOH             C   3H   6O   3     G  0300.00   5000.00  1000.00      1
 5.24778E+00    3.01153E-02   -1.20506E-05    2.14909E-09   -1.42781E-13       2
-2.76975E+04    1.70561E+00   -6.33411E+00    7.49355E-02   -8.02545E-05       3
 4.83008E-08   -1.14226E-11   -2.50730E+04    5.84283E+01                      4
C4H7O#3OOH             C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 1.33155E+01    2.57014E-02   -8.94224E-06    1.44189E-09   -8.90667E-14       2
-3.78807E+04   -4.09253E+01   -2.21978E+00    6.81655E-02   -4.19264E-05       3
 1.94646E-09    5.44409E-12   -3.38155E+04    3.88650E+01                      4
C4H7O#4OOH             C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 7.37224E+00    3.59340E-02   -1.39873E-05    2.44492E-09   -1.60057E-13       2
-3.23105E+04   -9.12457E+00   -6.94725E+00    8.74781E-02   -8.54724E-05       3
 4.59738E-08   -9.52539E-12   -2.89439E+04    6.18211E+01                      4
C4H7O#5OOH             C   4H   8O   3     G  0300.00   5000.00  1000.00      1
 1.60969E+01    2.12155E-02   -6.88753E-06    1.05753E-09   -6.31424E-14       2
-4.33055E+04   -5.60599E+01   -1.80129E+00    7.01810E-02   -4.46807E-05       3
 1.43750E-09    6.27377E-12   -3.86547E+04    3.57965E+01                      4
C7H13O#3OOH            C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 2.08484E+01    3.99818E-02   -1.32854E-05    2.07389E-09   -1.25261E-13       2
-3.98722E+04   -7.07112E+01    5.99701E+00    5.58105E-02    3.05823E-05       3
-7.28370E-08    3.00093E-11   -3.48568E+04    1.15530E+01                      4
C7H13O#4OOH            C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 1.34460E+01    5.48341E-02   -2.07439E-05    3.55300E-09   -2.29240E-13       2
-3.88029E+04   -3.32024E+01   -5.35213E+00    1.21491E-01   -1.16017E-04       3
 6.60846E-08   -1.54949E-11   -3.41554E+04    6.06026E+01                      4
C7H13O#5OOH            C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 2.30259E+01    3.80411E-02   -1.25930E-05    1.95965E-09   -1.18053E-13       2
-5.62632E+04   -8.84274E+01   -3.23332E+00    1.11881E-01   -7.60954E-05       3
 1.22607E-08    5.47954E-12   -4.94512E+04    4.60433E+01                      4
C7H13O#6OOH            C   7H  14O   3     G  0300.00   5000.00  1000.00      1
 2.30259E+01    3.80411E-02   -1.25930E-05    1.95965E-09   -1.18053E-13       2
-5.89806E+04   -9.11448E+01   -3.23332E+00    1.11881E-01   -7.60954E-05       3
 1.22607E-08    5.47954E-12   -5.21686E+04    4.33259E+01                      4
C5H9O2#4OOH            C   5H  10O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11O2#4OOH           C   6H  12O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11O2#5OOH           C   6H  12O   4     G  0300.00   5000.00  1000.00      1
 2.33568E+01    3.21563E-02   -1.04790E-05    1.61551E-09   -9.68522E-14       2
-7.20398E+04   -9.47283E+01   -5.28746E+00    1.19804E-01   -1.01273E-04       3
 3.44446E-08   -1.17572E-12   -6.49462E+04    5.02153E+01                      4
C6H11O2#3OOH           C   6H  12O   4     G  0300.00   5000.00  1000.00      1
 2.29930E+01    2.97672E-02   -9.04645E-06    1.32038E-09   -7.58521E-14       2
-6.47764E+04   -8.90730E+01   -3.11894E+00    8.98784E-02   -2.72467E-05       3
-3.70791E-08    2.25584E-11   -5.75804E+04    4.74319E+01                      4
C5H9O#3OOH             C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 1.53378E+01    3.16208E-02   -1.09769E-05    1.76807E-09   -1.09185E-13       2
-4.14018E+04   -4.97911E+01   -2.19462E+00    7.85070E-02   -4.54556E-05       3
-9.10780E-11    6.85420E-12   -3.67475E+04    4.05508E+01                      4
C5H9O#4OOH             C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 8.19608E+00    4.62262E-02   -1.86016E-05    3.33139E-09   -2.22038E-13       2
-4.04179E+04   -1.37681E+01   -1.07394E+01    1.25432E-01   -1.49261E-04       3
 9.89120E-08   -2.55894E-11   -3.63538E+04    7.76390E+01                      4
C5H9O#5OOH             C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 1.58289E+01    3.26267E-02   -1.17015E-05    1.92831E-09   -1.20978E-13       2
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-4.99408E+04   -5.49215E+01   -5.07720E+00    1.02068E-01   -9.49759E-05       3
 4.26077E-08   -6.13294E-12   -4.49647E+04    4.96319E+01                      4
C5H9O#6OOH              C   5H  10O   3     G  0300.00   5000.00  1000.00      1
 1.83319E+01    2.80820E-02   -9.51315E-06    1.50650E-09   -9.19620E-14       2
-4.66147E+04   -6.83924E+01   -1.03656E+00    8.67482E-02   -7.24921E-05       3
 2.81271E-08   -3.07806E-12   -4.16442E+04    3.00966E+01                      4
C4H8O2#4                C   4H   8O   2     G  0300.00   5000.00  1000.00      1
 5.00028E+00    3.74359E-02   -1.52063E-05    2.74101E-09   -1.83513E-13       2
-3.84709E+04   -5.80162E-01   -7.00474E+00    8.79144E-02   -1.03828E-04       3
 7.30203E-08   -2.04651E-11   -3.56779E+04    5.78241E+01                      4
C4H7O2#4OOH             C   4H   8O   4     G  0300.00   5000.00  1000.00      1
 9.98574E+00    3.53521E-02   -1.34975E-05    2.32765E-09   -1.50944E-13       2
-5.45055E+04   -2.07944E+01   -6.67986E+00    9.72310E-02   -1.00409E-04       3
 5.52251E-08   -1.14515E-11   -5.07730E+04    6.10971E+01                      4
R21C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.14133E+01    4.51599E-02   -1.49741E-05    2.33115E-09   -1.40377E-13       2
-4.78966E+03   -2.65924E+01   -4.88261E-01    8.28243E-02   -5.28756E-05       3
 1.38247E-08    5.14942E-13   -2.09090E+03    3.29121E+01                      4
R22C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.14133E+01    4.51599E-02   -1.49741E-05    2.33115E-09   -1.40377E-13       2
-4.78966E+03   -2.58993E+01   -4.88261E-01    8.28243E-02   -5.28756E-05       3
 1.38247E-08    5.14942E-13   -2.09090E+03    3.36052E+01                      4
R23C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.10659E+01    4.58305E-02   -1.53138E-05    2.40034E-09   -1.45412E-13       2
-4.70207E+03   -2.40787E+01    5.32519E-01    7.55898E-02   -3.66572E-05       3
-1.02378E-09    5.41567E-12   -2.18997E+03    2.93471E+01                      4
R24C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.17067E+01    4.52598E-02   -1.51004E-05    2.36259E-09   -1.42846E-13       2
-4.39088E+03   -2.78256E+01   -4.05559E-01    8.12875E-02   -4.65445E-05       3
 6.73079E-09    3.02532E-12   -1.53682E+03    3.32892E+01                      4
R25C5H11O               C   5H  11O   1     G  0300.00   5000.00  1000.00      1
 1.69994E+01    2.29874E-02   -6.45552E-06    8.88452E-10   -4.89064E-14       2
-1.83038E+04   -6.15910E+01   -2.15523E+00    8.13023E-02   -7.73437E-05       3
 4.23708E-08   -9.82108E-12   -1.30934E+04    3.64692E+01                      4
R26C5H11O               C   5H  11O   1     G  0300.00   5000.00  1000.00      1
 1.69994E+01    2.29874E-02   -6.45552E-06    8.88452E-10   -4.89064E-14       2
-2.22793E+04   -6.26895E+01   -2.15523E+00    8.13023E-02   -7.73437E-05       3
 4.23708E-08   -9.82108E-12   -1.70689E+04    3.53707E+01                      4
R27C6H13O               C   6H  13O   1     G  0300.00   5000.00  1000.00      1
 1.82538E+01    2.97172E-02   -8.74144E-06    1.24718E-09   -7.05733E-14       2
-2.29464E+04   -6.56650E+01    3.15798E+00    5.23691E-02    1.58046E-05       3
-5.54733E-08    2.46483E-11   -1.81221E+04    1.64155E+01                      4
R28C6H13O               C   6H  13O   1     G  0300.00   5000.00  1000.00      1
 1.76164E+01    3.02525E-02   -8.92589E-06    1.27725E-09   -7.24758E-14       2
-2.63325E+04   -6.30410E+01    4.00647E+00    4.72543E-02    2.40946E-05       3
-6.14704E-08    2.63764E-11   -2.18332E+04    1.17647E+01                      4
R29C6H13O               C   6H  13O   1     G  0300.00   5000.00  1000.00      1
 1.82538E+01    2.97172E-02   -8.74144E-06    1.24718E-09   -7.05733E-14       2
-2.28457E+04   -6.67635E+01    3.15798E+00    5.23691E-02    1.58046E-05       3
-5.54733E-08    2.46483E-11   -1.80215E+04    1.53170E+01                      4
R30C3H7OO               C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.36333E+01    1.35760E-02   -3.46244E-06    4.44745E-10   -2.33687E-14       2
-1.05995E+04   -4.33376E+01    6.21391E-01    4.71521E-02   -3.48428E-05       3
 1.31535E-08   -1.92195E-12   -6.71302E+03    2.48980E+01                      4
R31C4H9OO               C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.58522E+01    1.90655E-02   -5.20132E-06    7.01589E-10   -3.81205E-14       2
-1.41842E+04   -5.32522E+01    7.06940E-01    5.70736E-02   -3.73723E-05       3
 1.01403E-08   -1.76347E-13   -9.65133E+03    2.63331E+01                      4
R32C7H15OO              C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.22245E+01    3.63956E-02   -1.09858E-05    1.60073E-09   -9.21346E-14       2
-2.67877E+04   -8.22166E+01    4.81652E+00    6.12759E-02    1.81959E-05       3
-6.20088E-08    2.69397E-11   -2.10511E+04    1.30077E+01                      4
R33C7H15OO              C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.22245E+01    3.63956E-02   -1.09858E-05    1.60073E-09   -9.21346E-14       2
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-2.67877E+04   -8.15232E+01    4.81652E+00    6.12759E-02    1.81959E-05       3
-6.20088E-08    2.69397E-11   -2.10511E+04    1.37010E+01                      4
R34C7H15OO              C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.22620E+01    3.63273E-02   -1.09447E-05    1.59083E-09   -9.13062E-14       2
-2.68023E+04   -8.17296E+01    4.73145E+00    6.18732E-02    1.67470E-05       3
-6.05525E-08    2.64220E-11   -2.10421E+04    1.40614E+01                      4
R35C7H15OO              C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.22214E+01    3.61535E-02   -1.08394E-05    1.56900E-09   -8.97402E-14       2
-2.48427E+04   -8.14552E+01    9.25738E-01    8.71316E-02   -4.57361E-05       3
 1.93668E-09    4.74514E-12   -1.84627E+04    3.07892E+01                      4
R36C5H11                C   5H  11O   0     G  0300.00   5000.00  1000.00      1
 1.04169E+01    2.90697E-02   -9.09526E-06    1.35655E-09   -7.91737E-14       2
 1.50402E+03   -2.56497E+01   -5.21306E-01    6.12629E-02   -4.15561E-05       3
 1.34164E-08   -9.28586E-13    4.32085E+03    3.01384E+01                      4
R37C5H11OOO             C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.09204E+01    2.43084E-02   -6.81648E-06    9.37068E-10   -5.15375E-14       2
-3.59163E+04   -7.80044E+01   -2.53208E-01    8.25537E-02   -6.39146E-05       3
 2.33976E-08   -2.51219E-12   -2.99557E+04    3.16898E+01                      4
R38C5H11OOO             C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.07950E+01    2.35722E-02   -6.43984E-06    8.69397E-10   -4.72549E-14       2
-3.98836E+04   -7.93138E+01   -3.81562E+00    9.31177E-02   -7.20442E-05       3
 2.09254E-08    5.62902E-13   -3.33136E+04    4.71091E+01                      4
R39C4H9                 C   4H   9O   0     G  0300.00   5000.00  1000.00      1
 3.76329E+00    2.89493E-02   -9.48981E-06    1.46705E-09   -8.80017E-14       2
 2.79117E+03    7.16838E+00    1.13605E+00    2.60174E-02    1.77945E-05       3
-3.35124E-08    1.31525E-11    3.88634E+03    2.29561E+01                      4
R40C6H13OOO             C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.21706E+01    3.10663E-02   -9.13544E-06    1.30621E-09   -7.41937E-14       2
-4.05601E+04   -8.20666E+01    4.90895E+00    5.46615E-02    2.67708E-05       3
-7.20489E-08    3.11336E-11   -3.49676E+04    1.22739E+01                      4
R41C6H13OOO             C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.34017E+01    2.87213E-02   -8.10608E-06    1.12309E-09   -6.23013E-14       2
-4.62811E+04   -9.17803E+01   -4.23998E+00    1.05729E-01   -7.76311E-05       3
 1.86756E-08    2.53403E-12   -3.88759E+04    5.04161E+01                      4
R42C6H13OOO             C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.21936E+01    3.10255E-02   -9.11171E-06    1.30065E-09   -7.37400E-14       2
-4.05694E+04   -8.32943E+01    4.89376E+00    5.47646E-02    2.65277E-05       3
-7.18103E-08    3.10504E-11   -3.49660E+04    1.12394E+01                      4
R43C4H9O                C   4H   9O   1     G  0300.00   5000.00  1000.00      1
 1.39284E+01    1.88118E-02   -5.22435E-06    7.13668E-10   -3.91074E-14       2
-1.88841E+04   -5.02276E+01   -1.01455E+00    5.57244E-02   -3.35155E-05       3
 4.94447E-09    2.05505E-12   -1.44437E+04    2.82935E+01                      4
R44C3H6OOH              C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.38032E+01    1.25145E-02   -2.99567E-06    3.65614E-10   -1.84538E-14       2
-4.14957E+03   -4.01390E+01    1.79245E+00    4.81646E-02   -4.60604E-05       3
 2.62519E-08   -6.46414E-12   -7.91393E+02    2.16932E+01                      4
R45C3H6OOH              C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.43803E+01    1.20632E-02   -2.85506E-06    3.44577E-10   -1.72014E-14       2
-3.81445E+03   -4.35349E+01    8.95897E-01    5.35669E-02   -5.52210E-05       3
 3.32666E-08   -8.58837E-12   -1.42794E+02    2.54605E+01                      4
R46C4H8OOH              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.62621E+01    1.75288E-02   -4.51383E-06    5.82391E-10   -3.06082E-14       2
-7.77912E+03   -5.12759E+01    7.20942E-01    6.62556E-02   -6.70288E-05       3
 4.02798E-08   -1.03878E-11   -3.61590E+03    2.79664E+01                      4
R47C4H8OOH              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.60694E+01    1.79020E-02   -4.66799E-06    6.08503E-10   -3.22494E-14       2
-7.74922E+03   -5.03054E+01    1.73881E+00    5.90464E-02   -5.08822E-05       3
 2.55120E-08   -5.51809E-12   -3.71475E+03    2.37199E+01                      4
R48C4H8OOH              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.66395E+01    1.74604E-02   -4.53185E-06    5.88696E-10   -3.11177E-14       2
-7.41099E+03   -5.36611E+01    1.06688E+00    6.28975E-02   -5.63346E-05       3
 2.88426E-08   -6.34414E-12   -3.09028E+03    2.65350E+01                      4
R49C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29059E+01    3.43300E-02   -9.96700E-06    1.40537E-09   -7.86881E-14       2
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-2.04823E+04   -8.10343E+01    4.85686E+00    7.02784E-02   -1.10366E-05       3
-3.22859E-08    1.68738E-11   -1.50186E+04    1.52226E+01                      4
R50C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.26526E+01    3.48190E-02   -1.01926E-05    1.44776E-09   -8.15893E-14       2
-2.04302E+04   -7.97320E+01    6.13928E+00    6.12318E-02    9.52728E-06       3
-5.14643E-08    2.33042E-11   -1.51457E+04    9.85619E+00                      4
R51C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32071E+01    3.44045E-02   -1.00725E-05    1.43219E-09   -8.08477E-14       2
-2.00849E+04   -8.29988E+01    5.04730E+00    6.79950E-02   -2.91444E-06       3
-4.11645E-08    2.00146E-11   -1.44762E+04    1.44503E+01                      4
R52C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.26526E+01    3.48190E-02   -1.01926E-05    1.44776E-09   -8.15893E-14       2
-2.04302E+04   -7.97320E+01    6.13928E+00    6.12318E-02    9.52728E-06       3
-5.14643E-08    2.33042E-11   -1.51457E+04    9.85619E+00                      4
R53C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32071E+01    3.44045E-02   -1.00725E-05    1.43219E-09   -8.08477E-14       2
-2.00849E+04   -8.29988E+01    5.04730E+00    6.79950E-02   -2.91444E-06       3
-4.11645E-08    2.00146E-11   -1.44762E+04    1.44503E+01                      4
R54C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29059E+01    3.43300E-02   -9.96700E-06    1.40537E-09   -7.86881E-14       2
-2.04823E+04   -8.10343E+01    4.85686E+00    7.02784E-02   -1.10366E-05       3
-3.22859E-08    1.68738E-11   -1.50186E+04    1.52226E+01                      4
R55C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29059E+01    3.43300E-02   -9.96700E-06    1.40537E-09   -7.86881E-14       2
-2.04823E+04   -8.10343E+01    4.85686E+00    7.02784E-02   -1.10366E-05       3
-3.22859E-08    1.68738E-11   -1.50186E+04    1.52226E+01                      4
R56C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.26526E+01    3.48190E-02   -1.01926E-05    1.44776E-09   -8.15893E-14       2
-2.04302E+04   -7.97320E+01    6.13928E+00    6.12318E-02    9.52728E-06       3
-5.14643E-08    2.33042E-11   -1.51457E+04    9.85619E+00                      4
R57C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32071E+01    3.44045E-02   -1.00725E-05    1.43219E-09   -8.08477E-14       2
-2.00849E+04   -8.29988E+01    5.04730E+00    6.79950E-02   -2.91444E-06       3
-4.11645E-08    2.00146E-11   -1.44762E+04    1.44503E+01                      4
R58C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32705E+01    3.42913E-02   -1.00058E-05    1.41634E-09   -7.95409E-14       2
-2.15196E+04   -8.33529E+01    5.20962E+00    6.68709E-02   -2.17269E-07       3
-4.38548E-08    2.09663E-11   -1.59027E+04    1.37626E+01                      4
R59C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29026E+01    3.43356E-02   -9.97020E-06    1.40611E-09   -7.87477E-14       2
-2.04807E+04   -8.10152E+01    4.71400E+00    7.12660E-02   -1.34009E-05       3
-2.99339E-08    1.60440E-11   -1.50032E+04    1.58281E+01                      4
R60C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29059E+01    3.43300E-02   -9.96700E-06    1.40537E-09   -7.86881E-14       2
-2.04823E+04   -8.10343E+01    4.85686E+00    7.02784E-02   -1.10366E-05       3
-3.22859E-08    1.68738E-11   -1.50186E+04    1.52226E+01                      4
R61C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.29059E+01    3.43300E-02   -9.96700E-06    1.40537E-09   -7.86881E-14       2
-2.04823E+04   -8.10343E+01    4.85686E+00    7.02784E-02   -1.10366E-05       3
-3.22859E-08    1.68738E-11   -1.50186E+04    1.52226E+01                      4
R62C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.26526E+01    3.48190E-02   -1.01926E-05    1.44776E-09   -8.15893E-14       2
-2.04302E+04   -7.97320E+01    6.13928E+00    6.12318E-02    9.52728E-06       3
-5.14643E-08    2.33042E-11   -1.51457E+04    9.85619E+00                      4
R63C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.27788E+01    3.43127E-02   -9.95490E-06    1.40564E-09   -7.89325E-14       2
-1.84882E+04   -8.02760E+01    9.03075E-01    9.65757E-02   -7.60396E-05       3
 3.27376E-08   -5.70540E-12   -1.24234E+04    3.25784E+01                      4
R64C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.27788E+01    3.43127E-02   -9.95490E-06    1.40564E-09   -7.89325E-14       2
-1.84882E+04   -8.02760E+01    9.03075E-01    9.65757E-02   -7.60396E-05       3
 3.27376E-08   -5.70540E-12   -1.24234E+04    3.25784E+01                      4
R65C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.27020E+01    3.44497E-02   -1.00356E-05    1.42478E-09   -8.05088E-14       2
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-1.84573E+04   -7.98474E+01    7.60335E-01    9.75635E-02   -7.84072E-05       3
 3.50961E-08   -6.53860E-12   -1.24081E+04    3.31832E+01                      4
R66C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.27020E+01    3.44497E-02   -1.00356E-05    1.42478E-09   -8.05088E-14       2
-1.84573E+04   -7.98474E+01    7.60335E-01    9.75635E-02   -7.84072E-05       3
 3.50961E-08   -6.53860E-12   -1.24081E+04    3.31832E+01                      4
R67C5H11OO              C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.79703E+01    2.47591E-02   -7.07312E-06    9.89262E-10   -5.52761E-14       2
-1.77325E+04   -6.26185E+01    7.34943E-01    6.74032E-02   -4.09001E-05       3
 8.13765E-09    1.20766E-12   -1.25833E+04    2.80096E+01                      4
R68C5H11                C   5H  11O   0     G  0300.00   5000.00  1000.00      1
 9.80938E+00    2.95828E-02   -9.27552E-06    1.38666E-09   -8.11276E-14       2
 1.18013E+03   -2.20876E+01    1.26900E-01    5.75816E-02   -3.65250E-05       3
 1.05183E-08   -2.59295E-13    3.69904E+03    2.74231E+01                      4
R69C5H10OOOH            C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.17180E+01    2.26748E-02   -6.12615E-06    8.20093E-10   -4.42997E-14       2
-2.94972E+04   -7.77708E+01   -9.49232E-03    8.91976E-02   -8.48781E-05       3
 4.41249E-08   -9.40494E-12   -2.37346E+04    3.30757E+01                      4
R70C5H10OOOH            C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.17266E+01    2.26614E-02   -6.11936E-06    8.18701E-10   -4.41992E-14       2
-3.34764E+04   -7.85126E+01   -1.28977E-01    9.00202E-02   -8.68386E-05       3
 4.60662E-08   -1.00868E-11   -2.76972E+04    3.28895E+01                      4
R71C5H10OOOH            C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.15295E+01    2.20629E-02   -5.82810E-06    7.70750E-10   -4.14705E-14       2
-3.36937E+04   -7.83304E+01   -3.31555E+00    9.79662E-02   -8.86545E-05       3
 3.72722E-08   -4.76900E-12   -2.73713E+04    4.78176E+01                      4
R72C4H9OO               C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.64349E+01    1.86651E-02   -5.07409E-06    6.80833E-10   -3.67545E-14       2
-1.86292E+04   -6.02768E+01    3.56632E+00    3.85065E-02    1.13947E-05       3
-4.06792E-08    1.79361E-11   -1.44255E+04    9.83378E+00                      4
R73C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.30823E+01    2.92138E-02   -8.30957E-06    1.15803E-09   -6.45128E-14       2
-3.41842E+04   -8.24609E+01    5.22837E+00    6.07718E-02    7.10897E-06       3
-5.26384E-08    2.47122E-11   -2.87549E+04    1.33406E+01                      4
R74C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.25682E+01    2.95305E-02   -8.36599E-06    1.15799E-09   -6.39556E-14       2
-3.76197E+04   -8.08122E+01    6.14865E+00    5.51651E-02    1.65656E-05       3
-5.97857E-08    2.68428E-11   -3.24735E+04    8.09732E+00                      4
R75C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.30823E+01    2.92138E-02   -8.30957E-06    1.15803E-09   -6.45128E-14       2
-3.40835E+04   -8.38471E+01    5.22837E+00    6.07718E-02    7.10897E-06       3
-5.26384E-08    2.47122E-11   -2.86543E+04    1.19545E+01                      4
R76C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.41627E+01    2.71512E-02   -7.45256E-06    1.01496E-09   -5.58066E-14       2
-4.14074E+04   -9.27303E+01   -3.97337E+00    1.12208E-01   -9.81836E-05       3
 3.89828E-08   -4.20764E-12   -3.42175E+04    5.03180E+01                      4
R77C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.41627E+01    2.71512E-02   -7.45256E-06    1.01496E-09   -5.58066E-14       2
-4.00991E+04   -9.09387E+01   -3.97337E+00    1.12208E-01   -9.81836E-05       3
 3.89828E-08   -4.20764E-12   -3.29092E+04    5.21096E+01                      4
R78C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.27444E+01    2.91803E-02   -8.22279E-06    1.13491E-09   -6.26194E-14       2
-3.73900E+04   -8.20924E+01    5.01657E+00    6.31678E-02   -1.49024E-06       3
-4.31097E-08    2.12972E-11   -3.21108E+04    1.24219E+01                      4
R79C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.31283E+01    2.91323E-02   -8.26178E-06    1.14673E-09   -6.35840E-14       2
-3.39510E+04   -8.41032E+01    5.22837E+00    6.07718E-02    7.10897E-06       3
-5.26384E-08    2.47122E-11   -2.85033E+04    1.19545E+01                      4
R80C3H6OOOOH            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.90484E+01    1.26718E-02   -2.97004E-06    3.54256E-10   -1.74466E-14       2
-2.38740E+04   -6.50764E+01    2.13126E+00    5.97630E-02   -4.91660E-05       3
 1.81720E-08   -1.82122E-12   -1.91975E+04    2.23015E+01                      4
R81C3H6OOOOH            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.83522E+01    1.33235E-02   -3.20553E-06    3.94529E-10   -2.01319E-14       2
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-2.15524E+04   -6.02423E+01    2.64693E+00    5.58589E-02   -4.42549E-05       3
 1.66943E-08   -2.10627E-12   -1.70894E+04    2.13235E+01                      4
R82C4H8OOOOH            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13086E+01    1.80823E-02   -4.66794E-06    6.05601E-10   -3.20764E-14       2
-2.74729E+04   -7.45260E+01    2.02352E+00    7.10191E-02   -5.48767E-05       3
 1.82994E-08   -1.17364E-12   -2.21151E+04    2.52460E+01                      4
R83C4H8OOOOH            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13425E+01    1.80205E-02   -4.63077E-06    5.96639E-10   -3.13283E-14       2
-2.74865E+04   -7.47135E+01    2.18015E+00    6.99382E-02   -5.22933E-05       3
 1.57326E-08   -2.69049E-13   -2.21319E+04    2.45830E+01                      4
R84C4H8OOOOH            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.06546E+01    1.86580E-02   -4.85820E-06    6.34609E-10   -3.37925E-14       2
-2.51678E+04   -7.13117E+01    2.78837E+00    6.54017E-02   -4.58976E-05       3
 1.28194E-08   -6.40537E-14   -2.00338E+04    2.18256E+01                      4
R85C4H8OOH              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.62442E+01    1.75327E-02   -4.50884E-06    5.80404E-10   -3.04106E-14       2
-1.09468E+04   -5.11833E+01    8.38706E-01    6.54180E-02   -6.52570E-05       3
 3.87153E-08   -9.88741E-12   -6.79685E+03    2.74756E+01                      4
R86C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85688E+01    3.41897E-02   -9.89313E-06    1.39976E-09   -7.90204E-14       2
-4.05380E+04   -1.08665E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29549E+04    3.37796E+01                      4
R87C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
-4.05729E+04   -1.09160E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.52957E+01                      4
R88C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.78997E+04   -1.00773E+02    6.78748E+00    7.03730E-02    7.81416E-06       3
-5.74652E-08    2.63872E-11   -3.14218E+04    1.03497E+01                      4
R89C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.25381E+01    3.44040E-02   -9.95725E-06    1.40227E-09   -7.85285E-14       2
-2.43715E+04   -7.99258E+01    4.62134E+00    7.29023E-02   -1.97553E-05       3
-2.29980E-08    1.36357E-11   -1.90807E+04    1.49446E+01                      4
R90C5H10OOH             C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.88511E+01    2.32139E-02   -6.43357E-06    8.81636E-10   -4.86462E-14       2
-1.43463E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -1.00532E+04    9.81074E+00                      4
R91C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
-4.05729E+04   -1.09160E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.52957E+01                      4
R92C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57567E+00                      4
R93C5H10OOH             C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.84346E+01    2.30795E-02   -6.28662E-06    8.46957E-10   -4.59745E-14       2
-1.45207E+04   -6.09414E+01    8.08745E-01    7.61495E-02   -6.97504E-05       3
 3.76763E-08   -8.84439E-12   -9.72294E+03    2.93985E+01                      4
R94C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85688E+01    3.41897E-02   -9.89313E-06    1.39976E-09   -7.90204E-14       2
-4.05379E+04   -1.08665E+02    9.60741E-01    1.10162E-01   -8.01649E-05       3
 2.30258E-08    1.82638E-13   -3.29511E+04    3.39337E+01                      4
R95C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85688E+01    3.41897E-02   -9.89313E-06    1.39976E-09   -7.90204E-14       2
-4.05380E+04   -1.08665E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29549E+04    3.37797E+01                      4
R96C3H6OOH              C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.39619E+01    1.21787E-02   -2.85799E-06    3.42105E-10   -1.69417E-14       2
-7.34146E+03   -4.09293E+01    6.87659E-01    5.59501E-02   -6.38155E-05       3
 4.28124E-08   -1.20157E-11   -3.85151E+03    2.63165E+01                      4
R97C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
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-4.05729E+04   -1.09160E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.52957E+01                      4
R98C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.25381E+01    3.44040E-02   -9.95725E-06    1.40227E-09   -7.85285E-14       2
-2.43715E+04   -7.92327E+01    4.62134E+00    7.29023E-02   -1.97553E-05       3
-2.29980E-08    1.36357E-11   -1.90807E+04    1.56377E+01                      4
R99C4H8OOH              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.73307E+01    1.68294E-02   -4.31272E-06    5.53354E-10   -2.89074E-14       2
-1.11435E+04   -5.77842E+01    2.10196E-01    6.91274E-02   -6.67008E-05       3
 3.56004E-08   -7.86517E-12   -6.57046E+03    2.96529E+01                      4
R100C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.78997E+04   -1.00773E+02    6.75711E+00    7.05793E-02    7.32802E-06       3
-5.69880E-08    2.62208E-11   -3.14185E+04    1.04788E+01                      4
R101C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.88511E+01    2.32139E-02   -6.43357E-06    8.81636E-10   -4.86462E-14       2
-1.29373E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -8.64417E+03    9.81074E+00                      4
R102C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57598E+00                      4
R103C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32071E+01    3.44045E-02   -1.00725E-05    1.43219E-09   -8.08477E-14       2
-2.00849E+04   -8.29988E+01    5.04730E+00    6.79950E-02   -2.91444E-06       3
-4.11645E-08    2.00146E-11   -1.44762E+04    1.44503E+01                      4
R104C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
-4.05730E+04   -1.09162E+02    6.99703E-01    1.11973E-01   -8.45142E-05       3
 2.73628E-08   -1.35014E-12   -3.29232E+04    3.50389E+01                      4
R105C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85688E+01    3.41897E-02   -9.89313E-06    1.39976E-09   -7.90204E-14       2
-4.05379E+04   -1.07972E+02    9.60741E-01    1.10162E-01   -8.01649E-05       3
 2.30258E-08    1.82638E-13   -3.29511E+04    3.46268E+01                      4
R106C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85688E+01    3.41897E-02   -9.89313E-06    1.39976E-09   -7.90204E-14       2
-4.05380E+04   -1.07972E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29549E+04    3.44727E+01                      4
R107C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.22173E+01    3.50130E-02   -1.02532E-05    1.46132E-09   -8.28015E-14       2
-2.42923E+04   -7.75536E+01    5.82425E+00    6.44188E-02   -5.68825E-07       3
-4.07814E-08    1.95668E-11   -1.91994E+04    1.06062E+01                      4
R108C3H6OOH             C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.50332E+01    1.14968E-02   -2.67163E-06    3.16732E-10   -1.55368E-14       2
-7.53090E+03   -4.74429E+01    3.97669E-01    5.73200E-02   -5.96743E-05       3
 3.41718E-08   -8.05761E-12   -3.66142E+03    2.70592E+01                      4
R109C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
-4.05729E+04   -1.08467E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.59888E+01                      4
R110C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.72799E+01    1.69196E-02   -4.36563E-06    5.65862E-10   -2.99349E-14       2
-9.71418E+03   -5.75014E+01    2.65192E-01    6.87533E-02   -6.58213E-05       3
 3.47408E-08   -7.56690E-12   -5.16743E+03    2.94190E+01                      4
R111C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57590E+00                      4
R112C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.25313E+01    3.47927E-02   -1.01759E-05    1.44712E-09   -8.17730E-14       2
-1.84383E+04   -7.90055E+01    1.98283E+00    8.89205E-02   -5.87839E-05       3
 1.68305E-08   -4.22925E-13   -1.25287E+04    2.80722E+01                      4
R113C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.32059E+01    3.41618E-02   -9.92706E-06    1.40076E-09   -7.84769E-14       2
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-1.81409E+04   -8.29405E+01    1.02078E+00    9.47897E-02   -6.90957E-05       3
 2.50204E-08   -2.97103E-12   -1.18732E+04    3.21151E+01                      4
R114C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57583E+00                      4
R115C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57597E+00                      4
R116C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.27146E+01    3.44002E-02   -9.99971E-06    1.41553E-09   -7.97165E-14       2
-2.16372E+04   -7.99247E+01    7.91185E-01    9.73201E-02   -7.80412E-05       3
 3.49147E-08   -6.52127E-12   -1.55797E+04    3.30617E+01                      4
R117C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.79001E+04   -1.01466E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57645E+00                      4
R118C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.84879E+01    2.30118E-02   -6.25367E-06    8.39882E-10   -4.54220E-14       2
-1.13669E+04   -6.12307E+01    6.25544E-01    7.74532E-02   -7.26708E-05       3
 4.04136E-08   -9.76785E-12   -6.53517E+03    3.01646E+01                      4
R119C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.84879E+01    2.30118E-02   -6.25367E-06    8.39882E-10   -4.54220E-14       2
-1.13669E+04   -6.12307E+01    6.25544E-01    7.74532E-02   -7.26708E-05       3
 4.04136E-08   -9.76785E-12   -6.53517E+03    3.01646E+01                      4
R120C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.82338E+01    2.34979E-02   -6.47570E-06    8.81811E-10   -4.83334E-14       2
-1.13135E+04   -5.99212E+01    1.86607E+00    6.86882E-02   -5.27615E-05       3
 2.18688E-08   -3.55540E-12   -6.65767E+03    2.49768E+01                      4
R121C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.88283E+01    2.30126E-02   -6.31408E-06    8.56215E-10   -4.67477E-14       2
-1.09849E+04   -6.34124E+01    1.10965E+00    7.31303E-02   -5.96440E-05       3
 2.66359E-08   -4.89249E-12   -6.02423E+03    2.81490E+01                      4
R122C5H11OO             C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.81178E+01    2.47389E-02   -7.06253E-06    9.83639E-10   -5.45979E-14       2
-1.97350E+04   -6.34893E+01    4.90551E+00    3.96065E-02    2.76933E-05       3
-6.04584E-08    2.50473E-11   -1.52016E+04    9.73754E+00                      4
R123C5H10OOOOOH         C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.58868E+01    2.36053E-02   -6.31044E-06    8.34731E-10   -4.45198E-14       2
-4.72128E+04   -9.55877E+01    1.87200E+00    9.06290E-02   -7.19826E-05       3
 2.57919E-08   -2.36211E-12   -4.05949E+04    2.83735E+01                      4
R124C5H10OOOOOH         C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.57188E+01    2.29845E-02   -6.03515E-06    7.94627E-10   -4.26241E-14       2
-5.11683E+04   -9.69641E+01   -1.55164E+00    1.00210E-01   -7.77064E-05       3
 2.08825E-08    1.58401E-12   -4.39675E+04    4.29207E+01                      4
R125C5H10OOOH           C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.13414E+01    2.27145E-02   -6.08451E-06    8.07745E-10   -4.32887E-14       2
-3.29400E+04   -7.67831E+01   -2.78481E-01    9.19893E-02   -9.44234E-05       3
 5.45928E-08   -1.31504E-11   -2.73360E+04    3.28046E+01                      4
R126C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.57188E+01    1.81300E-02   -4.72802E-06    6.15839E-10   -3.25887E-14       2
-1.06464E+04   -5.01470E+01    2.02910E+00    5.56390E-02   -4.29719E-05       3
 1.78446E-08   -2.81018E-12   -6.71492E+03    2.09829E+01                      4
R127C5H10OOOOOH         C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.57188E+01    2.29845E-02   -6.03515E-06    7.94627E-10   -4.26241E-14       2
-5.14198E+04   -9.69635E+01   -1.58925E+00    1.00469E-01   -7.83252E-05       3
 2.14963E-08    1.36804E-12   -4.42151E+04    4.30806E+01                      4
R128C5H10OOOH           C   5H  11O   3     G  0300.00   5000.00  1000.00      1
 2.11436E+01    2.21171E-02   -5.79364E-06    7.59643E-10   -4.05253E-14       2
-3.71323E+04   -7.76958E+01   -3.54147E+00    1.00476E-01   -9.75638E-05       3
 4.71422E-08   -8.31439E-12   -3.09776E+04    4.69563E+01                      4
R129C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.72144E+01    1.70748E-02   -4.41399E-06    5.70281E-10   -2.99530E-14       2
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-1.19538E+04   -5.95444E+01    3.78554E+00    4.53128E-02   -9.94330E-06       3
-1.95904E-08    1.09188E-11   -7.95045E+03    1.17284E+01                      4
R130C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.72417E+01    3.01750E-02   -8.52020E-06    1.18037E-09   -6.54492E-14       2
-5.18996E+04   -1.00927E+02    7.04235E+00    6.26457E-02    1.90264E-05       3
-7.01013E-08    3.14870E-11   -4.56079E+04    8.23322E+00                      4
R131C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84984E+01    2.78124E-02   -7.50721E-06    1.00315E-09   -5.40576E-14       2
-5.76322E+04   -1.10386E+02   -2.20293E+00    1.14416E-01   -8.71710E-05       3
 2.25469E-08    2.15633E-12   -4.95062E+04    4.71852E+01                      4
R132C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.27121E+01    2.92395E-02   -8.25848E-06    1.14354E-09   -6.33408E-14       2
-3.76290E+04   -8.08147E+01    5.01657E+00    6.31678E-02   -1.49024E-06       3
-4.31097E-08    2.12972E-11   -3.23624E+04    1.35204E+01                      4
R133C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.72417E+01    3.01750E-02   -8.52020E-06    1.18037E-09   -6.54492E-14       2
-5.18996E+04   -1.00928E+02    7.04235E+00    6.26457E-02    1.90264E-05       3
-7.01013E-08    3.14870E-11   -4.56079E+04    8.23308E+00                      4
R134C4H8OOOH             C   4H   9O   3     G  0300.00   5000.00  1000.00      1
 1.81363E+01    1.91712E-02   -5.17319E-06    6.94981E-10   -3.78072E-14       2
-2.79830E+04   -6.30154E+01    4.02409E+00    4.42356E-02    3.50601E-06       3
-3.56077E-08    1.66905E-11   -2.35661E+04    1.29832E+01                      4
R135C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84889E+01    2.78279E-02   -7.51552E-06    1.00496E-09   -5.41961E-14       2
-5.78796E+04   -1.11433E+02   -2.27044E+00    1.14884E-01   -8.82956E-05       3
 2.36694E-08    1.75909E-12   -4.97506E+04    4.63707E+01                      4
R136C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84889E+01    2.78279E-02   -7.51552E-06    1.00496E-09   -5.41961E-14       2
-5.78796E+04   -1.10334E+02   -2.27044E+00    1.14884E-01   -8.82956E-05       3
 2.36694E-08    1.75909E-12   -4.97506E+04    4.74690E+01                      4
R137C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.33875E+01    2.73804E-02   -7.41145E-06    9.91443E-10   -5.34131E-14       2
-4.42915E+04   -8.84801E+01   -3.65822E+00    1.11828E-01   -1.03498E-04       3
 4.69951E-08   -7.34981E-12   -3.74822E+04    4.84306E+01                      4
R138C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84889E+01    2.78279E-02   -7.51552E-06    1.00496E-09   -5.41961E-14       2
-5.73764E+04   -1.11433E+02   -2.27044E+00    1.14884E-01   -8.82956E-05       3
 2.36694E-08    1.75909E-12   -4.92474E+04    4.63706E+01                      4
R139C6H12OOOOOH          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.72417E+01    3.01750E-02   -8.52020E-06    1.18037E-09   -6.54492E-14       2
-5.16479E+04   -1.00926E+02    6.95194E+00    6.32675E-02    1.75456E-05       3
-6.86351E-08    3.09718E-11   -4.53465E+04    8.61737E+00                      4
R140C6H12OOOH            C   6H  13O   3     G  0300.00   5000.00  1000.00      1
 2.27444E+01    2.91803E-02   -8.22279E-06    1.13491E-09   -6.26194E-14       2
-3.73900E+04   -8.20924E+01    5.01657E+00    6.31678E-02   -1.49024E-06       3
-4.31097E-08    2.12972E-11   -3.21108E+04    1.24219E+01                      4
R141C3H5O4H2             C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.96232E+01    1.14809E-02   -2.55679E-06    2.98006E-10   -1.47001E-14       2
-1.84325E+04   -6.43222E+01    2.38352E+00    6.63420E-02   -6.99612E-05       3
 3.87209E-08   -8.64785E-12   -1.40344E+04    2.29569E+01                      4
R142C3H5O4H2             C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.92159E+01    1.15789E-02   -2.55038E-06    2.93264E-10   -1.42464E-14       2
-2.05556E+04   -6.17800E+01    2.21088E+00    6.84598E-02   -7.78745E-05       3
 4.75472E-08   -1.18084E-11   -1.63376E+04    2.36648E+01                      4
R143C3H6OOOOH            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.89993E+01    1.27598E-02   -3.02203E-06    3.66603E-10   -1.84641E-14       2
-2.38547E+04   -6.48045E+01    2.22168E+00    5.91333E-02   -4.76472E-05       3
 1.66500E-08   -1.28068E-12   -1.92071E+04    2.19180E+01                      4
R144C3H5O4H2             C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.86564E+01    1.20124E-02   -2.66397E-06    3.05834E-10   -1.47197E-14       2
-1.51135E+04   -5.90838E+01    2.77259E+00    6.42763E-02   -7.20994E-05       3
 4.50478E-08   -1.16929E-11   -1.10664E+04    2.10972E+01                      4
R145C3H5O4H2             C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.86145E+01    1.20586E-02   -2.68371E-06    3.09714E-10   -1.50061E-14       2
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-1.82713E+04   -5.81637E+01    2.77472E+00    6.42366E-02   -7.22327E-05       3
 4.53731E-08   -1.18572E-11   -1.42349E+04    2.17897E+01                      4
R146C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.16583E+01    1.66426E-02   -4.03698E-06    4.97321E-10   -2.52477E-14       2
-2.42227E+04   -7.29239E+01    2.20815E+00    7.89997E-02   -8.18940E-05       3
 4.60137E-08   -1.05816E-11   -1.92666E+04    2.54712E+01                      4
R147C4H8OOOOH          C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13086E+01    1.80823E-02   -4.66794E-06    6.05601E-10   -3.20764E-14       2
-2.74729E+04   -7.52194E+01    2.02352E+00    7.10191E-02   -5.48767E-05       3
 1.82994E-08   -1.17364E-12   -2.21151E+04    2.45526E+01                      4
R148C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.15049E+01    1.69702E-02   -4.17015E-06    5.19569E-10   -2.66380E-14       2
-2.10329E+04   -7.21631E+01    3.09177E+00    7.27500E-02   -6.78306E-05       3
 3.31390E-08   -6.33435E-12   -1.61829E+04    2.17843E+01                      4
R149C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.20287E+01    1.66136E-02   -4.08531E-06    5.11885E-10   -2.64962E-14       2
-2.06767E+04   -7.52627E+01    2.40013E+00    7.67323E-02   -7.35851E-05       3
 3.67595E-08   -7.25945E-12   -1.55562E+04    2.46836E+01                      4
R150C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.21127E+01    1.64634E-02   -3.99663E-06    4.90819E-10   -2.47593E-14       2
-2.21194E+04   -7.57309E+01    2.48722E+00    7.61268E-02   -7.21273E-05       3
 3.53016E-08   -6.74263E-12   -1.69745E+04    2.43150E+01                      4
R151C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.16246E+01    1.67315E-02   -4.09709E-06    5.12477E-10   -2.65372E-14       2
-2.10347E+04   -7.27301E+01    2.23817E+00    7.88288E-02   -8.12855E-05       3
 4.52443E-08   -1.02699E-11   -1.61017E+04    2.53339E+01                      4
R152C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.16460E+01    1.66647E-02   -4.05014E-06    5.00471E-10   -2.55091E-14       2
-2.42178E+04   -7.28556E+01    2.18145E+00    7.91801E-02   -8.23160E-05       3
 4.64249E-08   -1.07241E-11   -1.92637E+04    2.55849E+01                      4
R153C4H8OOOOH          C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13988E+01    1.79214E-02   -4.57328E-06    5.83203E-10   -3.02363E-14       2
-2.75092E+04   -7.50297E+01    2.20696E+00    6.97604E-02   -5.18888E-05       3
 1.53527E-08   -1.42676E-13   -2.21349E+04    2.44667E+01                      4
R154C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.10358E+01    1.71875E-02   -4.21543E-06    5.24547E-10   -2.68738E-14       2
-1.87547E+04   -6.91822E+01    2.71540E+00    7.51980E-02   -7.70546E-05       3
 4.44777E-08   -1.08192E-11   -1.39896E+04    2.38270E+01                      4
R155C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.10167E+01    1.71931E-02   -4.21120E-06    5.22715E-10   -2.66876E-14       2
-2.19215E+04   -6.90817E+01    2.69095E+00    7.53338E-02   -7.75900E-05       3
 4.51878E-08   -1.11150E-11   -1.71551E+04    2.39403E+01                      4
R156C4H8OOOOH          C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.05415E+01    1.80030E-02   -4.53742E-06    5.78020E-10   -3.02113E-14       2
-3.01393E+04   -7.19938E+01    3.71506E+00    4.83888E-02    7.31255E-06       3
-4.64042E-08    2.16193E-11   -2.50401E+04    1.81770E+01                      4
R157C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R158C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R159C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.88523E+01    3.22737E-02   -8.91902E-06    1.21302E-09   -6.62078E-14       2
-3.81142E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09648E+04    3.65169E+01                      4
R160C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91717E+01    3.22852E-02   -8.97894E-06    1.22838E-09   -6.74118E-14       2
-3.42054E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R161C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
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-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R162C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R163C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.52345E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78004E+04    3.40991E+01                      4
R164C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
-3.41879E+04   -1.07508E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R165C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.88523E+01    3.22737E-02   -8.91902E-06    1.21302E-09   -6.62078E-14       2
-3.81142E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09648E+04    3.65169E+01                      4
R166C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91717E+01    3.22852E-02   -8.97894E-06    1.22838E-09   -6.74118E-14       2
-3.42054E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R167C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R168C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R169C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R170C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.74760E+01    3.37455E-02   -9.47188E-06    1.30571E-09   -7.21030E-14       2
-3.54057E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94435E+04    1.19254E+01                      4
R171C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
-3.15214E+04   -9.99147E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R172C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.49617E+01    3.94638E-02   -1.20690E-05    1.77277E-09   -1.02475E-13       2
-4.39241E+04   -9.24963E+01    4.32434E+00    7.49541E-02    1.04280E-05       3
-6.71421E-08    3.15396E-11   -3.76306E+04    1.83837E+01                      4
R173C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07598E+04   -8.21560E+01    6.87268E+00    4.87349E-02    1.72258E-05       3
-5.58217E-08    2.44602E-11   -2.55724E+04    5.70996E+00                      4
R174C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.83758E+01    2.34866E-02   -6.46999E-06    8.77511E-10   -4.77816E-14       2
-1.33135E+04   -6.07627E+01    6.00935E+00    4.10908E-02    1.53302E-05       3
-4.62069E-08    2.00942E-11   -9.27325E+03    6.81659E+00                      4
R175C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.88511E+01    2.32139E-02   -6.43357E-06    8.81636E-10   -4.86462E-14       2
-1.29373E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -8.64417E+03    9.81074E+00                      4
R176C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.52345E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78004E+04    3.40991E+01                      4
R177C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.87936E+01    3.23799E-02   -8.98240E-06    1.22822E-09   -6.74697E-14       2
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-3.80908E+04   -1.05890E+02    3.87168E-01    1.24423E-01   -1.24462E-04       3
 6.83835E-08   -1.53706E-11   -3.09407E+04    3.74722E+01                      4
R178C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91717E+01    3.22852E-02   -8.97894E-06    1.22838E-09   -6.74118E-14       2
-3.42054E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R179C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91717E+01    3.22852E-02   -8.97894E-06    1.22838E-09   -6.74118E-14       2
-3.42054E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R180C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R181C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R182C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.74760E+01    3.37455E-02   -9.47188E-06    1.30571E-09   -7.21030E-14       2
-3.54057E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94435E+04    1.19254E+01                      4
R183C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
-3.15214E+04   -9.99147E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R184C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
-3.15214E+04   -9.99147E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R185C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.28367E+01    2.33575E-02   -6.20296E-06    8.19372E-10   -4.38163E-14       2
-3.37534E+04   -8.23343E+01    3.73843E+00    5.87407E-02    3.75044E-06       3
-4.83857E-08    2.29984E-11   -2.79717E+04    1.98730E+01                      4
R186C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.88523E+01    3.22737E-02   -8.91902E-06    1.21302E-09   -6.62078E-14       2
-3.81142E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09648E+04    3.65169E+01                      4
R187C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R188C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R189C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
-3.41879E+04   -1.08201E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.55087E+01                      4
R190C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.88523E+01    3.22737E-02   -8.91902E-06    1.21302E-09   -6.62078E-14       2
-3.81142E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09648E+04    3.65169E+01                      4
R191C3H6OOOOH           C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.85324E+01    1.23522E-02   -2.78554E-06    3.22750E-10   -1.55710E-14       2
-2.66995E+04   -6.33782E+01    1.33640E+00    5.39201E-02   -2.58051E-05       3
-9.63113E-09    8.61200E-12   -2.18514E+04    2.65104E+01                      4
R192C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.52345E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78004E+04    3.40991E+01                      4
R193C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
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-3.41879E+04   -1.07508E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R194C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
-3.41879E+04   -1.07508E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R195C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.88523E+01    3.22737E-02   -8.91902E-06    1.21302E-09   -6.62078E-14       2
-3.81142E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09648E+04    3.65169E+01                      4
R196C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41690E+04   -1.06681E+02    2.01569E+00    1.11984E-01   -9.33320E-05       3
 3.80733E-08   -5.04990E-12   -2.70175E+04    3.12226E+01                      4
R197C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.49617E+01    3.94638E-02   -1.20690E-05    1.77277E-09   -1.02475E-13       2
-4.39241E+04   -9.18031E+01    4.32434E+00    7.49541E-02    1.04280E-05       3
-6.71421E-08    3.15396E-11   -3.76306E+04    1.90768E+01                      4
R198C4H9OO              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.65218E+01    1.84696E-02   -5.00119E-06    6.70789E-10   -3.62951E-14       2
-1.64980E+04   -5.72510E+01   -1.15391E-01    6.30619E-02   -4.71494E-05       3
 1.63007E-08   -1.48274E-12   -1.17258E+04    2.93080E+01                      4
R199C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R200C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R201C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78572E+01    3.36449E-02   -9.46464E-06    1.30479E-09   -7.19397E-14       2
-3.15214E+04   -9.99164E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R202C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.74760E+01    3.37455E-02   -9.47188E-06    1.30571E-09   -7.21030E-14       2
-3.54057E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94435E+04    1.19254E+01                      4
R203C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07596E+04   -8.14626E+01    6.74655E+00    4.96086E-02    1.51304E-05       3
-5.37340E-08    2.37228E-11   -2.55588E+04    6.93703E+00                      4
R204C5H11OO             C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.81178E+01    2.47389E-02   -7.06253E-06    9.83639E-10   -5.45979E-14       2
-1.97346E+04   -6.41822E+01    4.68790E+00    4.11153E-02    2.40717E-05       3
-5.68472E-08    2.37708E-11   -1.51784E+04    9.96529E+00                      4
R205C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.83758E+01    2.34866E-02   -6.46999E-06    8.77511E-10   -4.77816E-14       2
-1.33135E+04   -6.07627E+01    6.00935E+00    4.10908E-02    1.53302E-05       3
-4.62069E-08    2.00942E-11   -9.27325E+03    6.81659E+00                      4
R206C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.74760E+01    3.37455E-02   -9.47188E-06    1.30571E-09   -7.21030E-14       2
-3.54057E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94435E+04    1.19254E+01                      4
R207C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78572E+01    3.36449E-02   -9.46464E-06    1.30479E-09   -7.19397E-14       2
-3.15214E+04   -9.99164E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R208C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
-3.15214E+04   -9.99147E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R209C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
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-3.15214E+04   -9.99147E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R210C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
-3.78997E+04   -1.01466E+02    6.75711E+00    7.05793E-02    7.32802E-06       3
-5.69880E-08    2.62208E-11   -3.14185E+04    9.78564E+00                      4
R211C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85929E+01    3.27699E-02   -9.14712E-06    1.25623E-09   -6.92081E-14       2
-3.80583E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10552E+04    3.26031E+01                      4
R212C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R213C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R214C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85929E+01    3.27699E-02   -9.14712E-06    1.25623E-09   -6.92081E-14       2
-3.80583E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10552E+04    3.26031E+01                      4
R215C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38255E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.63914E+04    3.40991E+01                      4
R216C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85929E+01    3.27699E-02   -9.14712E-06    1.25623E-09   -6.92081E-14       2
-3.80583E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10552E+04    3.26031E+01                      4
R217C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.49516E+01    3.94815E-02   -1.20793E-05    1.77519E-09   -1.02673E-13       2
-4.39199E+04   -9.17462E+01    4.27237E+00    7.53196E-02    9.53843E-06       3
-6.62436E-08    3.12183E-11   -3.76251E+04    1.92965E+01                      4
R218C3H7OO              C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.42941E+01    1.29920E-02   -3.26734E-06    4.14434E-10   -2.15322E-14       2
-1.29085E+04   -4.79776E+01   -1.26900E-01    5.26375E-02   -4.34523E-05       3
 1.82031E-08   -2.85659E-12   -8.79550E+03    2.68651E+01                      4
R219C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.52345E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78004E+04    3.40991E+01                      4
R220C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
-3.41879E+04   -1.07508E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.62018E+01                      4
R221C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.91286E+01    3.23605E-02   -9.02255E-06    1.23857E-09   -6.82405E-14       2
-3.41879E+04   -1.08201E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69002E+04    3.55087E+01                      4
R222C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.85929E+01    3.27699E-02   -9.14712E-06    1.25623E-09   -6.92081E-14       2
-3.80583E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10552E+04    3.26031E+01                      4
R223C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77754E+01    3.37641E-02   -9.52839E-06    1.31925E-09   -7.31055E-14       2
-3.46641E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85845E+04    1.01360E+01                      4
R224C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.75668E+01    3.41971E-02   -9.72611E-06    1.35581E-09   -7.55721E-14       2
-3.14537E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55055E+04    6.26062E+00                      4
R225C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.73677E+01    3.53503E-02   -1.02628E-05    1.44821E-09   -8.11952E-14       2
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-3.79002E+04   -1.01465E+02    7.07308E+00    6.83986E-02    1.25408E-05       3
-6.21674E-08    2.80462E-11   -3.14525E+04    8.44847E+00                      4
R226C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.72275E+01    3.53565E-02   -1.02639E-05    1.45153E-09   -8.16895E-14       2
-3.59006E+04   -9.99421E+01    2.87463E+00    9.63752E-02   -5.64548E-05       3
 6.80405E-09    4.08129E-12   -2.88309E+04    2.75332E+01                      4
R227C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77754E+01    3.37641E-02   -9.52839E-06    1.31925E-09   -7.31055E-14       2
-3.46641E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85845E+04    1.01360E+01                      4
R228C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.75668E+01    3.41971E-02   -9.72611E-06    1.35581E-09   -7.55721E-14       2
-3.14537E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55055E+04    6.26062E+00                      4
R229C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.11339E+04   -1.02024E+02    7.12280E+00    7.63821E-02   -1.16257E-05       3
-3.82570E-08    2.00314E-11   -2.48587E+04    9.96241E+00                      4
R230C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.75668E+01    3.41971E-02   -9.72611E-06    1.35581E-09   -7.55721E-14       2
-3.14537E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55055E+04    6.26062E+00                      4
R231C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.11339E+04   -1.02024E+02    7.12280E+00    7.63821E-02   -1.16257E-05       3
-3.82570E-08    2.00314E-11   -2.48587E+04    9.96241E+00                      4
R232C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77754E+01    3.37641E-02   -9.52839E-06    1.31925E-09   -7.31055E-14       2
-3.46641E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85845E+04    1.01360E+01                      4
R233C7H14OOOOH          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.72831E+01    3.43728E-02   -9.73595E-06    1.34713E-09   -7.43680E-14       2
-4.09342E+04   -1.02242E+02    3.82351E+00    7.91990E-02   -2.82992E-06       3
-5.28530E-08    2.59241E-11   -3.38394E+04    2.30989E+01                      4
R234C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.75668E+01    3.41971E-02   -9.72611E-06    1.35581E-09   -7.55721E-14       2
-3.14537E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55055E+04    6.26062E+00                      4
R235C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.11339E+04   -1.02024E+02    7.12280E+00    7.63821E-02   -1.16257E-05       3
-3.82570E-08    2.00314E-11   -2.48587E+04    9.96241E+00                      4
R236C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77754E+01    3.37641E-02   -9.52839E-06    1.31925E-09   -7.31055E-14       2
-3.46641E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85845E+04    1.01360E+01                      4
R237C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07598E+04   -8.21559E+01    6.87268E+00    4.87349E-02    1.72258E-05       3
-5.58217E-08    2.44602E-11   -2.55724E+04    5.71007E+00                      4
R238C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07598E+04   -8.21553E+01    6.83506E+00    4.89942E-02    1.66070E-05       3
-5.52080E-08    2.42443E-11   -2.55683E+04    5.86989E+00                      4
R239C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07597E+04   -8.21540E+01    6.81264E+00    4.91504E-02    1.62312E-05       3
-5.48328E-08    2.41115E-11   -2.55659E+04    5.96597E+00                      4
R240C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30002E+01    2.39361E-02   -6.48531E-06    8.66379E-10   -4.65319E-14       2
-2.88052E+04   -8.12487E+01    3.01512E+00    7.43746E-02   -4.62199E-05       3
 7.66715E-09    2.41829E-12   -2.29877E+04    2.33490E+01                      4
R241C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.85259E+01    2.31877E-02   -6.35918E-06    8.62221E-10   -4.70834E-14       2
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-1.33262E+04   -6.14952E+01    5.09002E+00    4.76127E-02    8.43541E-07       3
-3.31039E-08    1.58162E-11   -9.18490E+03    1.06463E+01                      4
R242C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.66507E+01    2.20454E-02   -5.66922E-06    7.28439E-10   -3.80446E-14       2
-4.07832E+04   -9.72521E+01    2.02530E+00    9.78957E-02   -9.44323E-05       3
 4.79943E-08   -9.77445E-12   -3.43644E+04    2.80645E+01                      4
R243C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.61586E+01    2.22899E-02   -5.74706E-06    7.43923E-10   -3.92843E-14       2
-4.41796E+04   -9.35413E+01    1.83759E+00    1.00121E-01   -1.02613E-04       3
 5.70956E-08   -1.30350E-11   -3.79745E+04    2.95288E+01                      4
R244C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.65739E+01    2.21831E-02   -5.75052E-06    7.47746E-10   -3.96352E-14       2
-4.47287E+04   -9.75191E+01    2.33558E+00    9.57316E-02   -8.92058E-05       3
 4.27524E-08   -7.91178E-12   -3.83729E+04    2.60591E+01                      4
R245C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.65756E+01    2.12662E-02   -5.30338E-06    6.65977E-10   -3.42151E-14       2
-4.47774E+04   -9.70707E+01   -1.38208E+00    1.07371E-01   -9.99195E-05       3
 4.28630E-08   -5.75404E-12   -3.77390E+04    4.46211E+01                      4
R246C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.61337E+01    2.14232E-02   -5.33076E-06    6.69543E-10   -3.44735E-14       2
-4.81949E+04   -9.50288E+01   -1.23661E+00    1.07281E-01   -1.02528E-04       3
 4.63952E-08   -7.04204E-12   -4.13846E+04    4.32890E+01                      4
R247C5H10OOOOOH         C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.60876E+01    2.26188E-02   -5.89432E-06    7.69352E-10   -4.08827E-14       2
-5.23754E+04   -9.95446E+01   -2.18086E-01    9.39955E-02   -6.59429E-05       3
 1.14390E-08    4.27516E-12   -4.52725E+04    3.61804E+01                      4
R248C4H8OOOOH           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.12733E+01    1.81942E-02   -4.69529E-06    6.05599E-10   -3.17543E-14       2
-2.96275E+04   -7.74386E+01    5.63013E+00    4.69489E-02    2.61001E-06       3
-3.77523E-08    1.79632E-11   -2.48063E+04    6.50062E+00                      4
R249C4H9OO              C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.60581E+01    1.88766E-02   -5.14021E-06    6.92880E-10   -3.76552E-14       2
-1.53281E+04   -5.58326E+01    5.76065E-02    5.93770E-02   -3.93844E-05       3
 1.02650E-08    1.27553E-13   -1.05891E+04    2.80846E+01                      4
R250C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.61337E+01    2.14232E-02   -5.33076E-06    6.69543E-10   -3.44735E-14       2
-4.81949E+04   -9.50288E+01   -1.23661E+00    1.07281E-01   -1.02528E-04       3
 4.63952E-08   -7.04204E-12   -4.13846E+04    4.32890E+01                      4
R251C5H10OOOOOH         C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R252C4H8OOOOH           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.12733E+01    1.81942E-02   -4.69529E-06    6.05599E-10   -3.17543E-14       2
-2.96275E+04   -7.74389E+01    5.61494E+00    4.70521E-02    2.36694E-06       3
-3.75137E-08    1.78800E-11   -2.48047E+04    6.56493E+00                      4
R253C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.80950E+01    2.84406E-02   -7.77012E-06    1.04949E-09   -5.70945E-14       2
-4.55030E+04   -1.02389E+02    7.35346E+00    6.88038E-02   -7.26991E-07       3
-5.06200E-08    2.50466E-11   -3.93941E+04    7.95115E+00                      4
R254C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.76572E+01    2.85864E-02   -7.78927E-06    1.05129E-09   -5.72310E-14       2
-4.89204E+04   -9.89789E+01    6.96677E+00    7.24180E-02   -1.22620E-05       3
-3.81540E-08    2.05905E-11   -4.29830E+04    1.02570E+01                      4
R255C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.74814E+01    2.89314E-02   -7.92741E-06    1.07319E-09   -5.84845E-14       2
-4.88976E+04   -9.94896E+01    7.98304E+00    6.52074E-02    3.91670E-06       3
-5.29791E-08    2.54879E-11   -4.30815E+04    4.63285E+00                      4
R256C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.80950E+01    2.84406E-02   -7.77012E-06    1.04949E-09   -5.70945E-14       2
-4.54023E+04   -1.03082E+02    7.35346E+00    6.88038E-02   -7.26991E-07       3
-5.06200E-08    2.50466E-11   -3.92935E+04    7.25807E+00                      4
R257C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92913E+01    2.61976E-02   -6.83236E-06    8.89020E-10   -4.69549E-14       2
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-5.25227E+04   -1.10829E+02   -1.67207E+00    1.19056E-01   -1.03293E-04       3
 3.84188E-08   -3.01181E-12   -4.46244E+04    4.66622E+01                      4
R258C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92913E+01    2.61976E-02   -6.83236E-06    8.89020E-10   -4.69549E-14       2
-5.12143E+04   -1.10135E+02   -1.67207E+00    1.19056E-01   -1.03293E-04       3
 3.84188E-08   -3.01181E-12   -4.33160E+04    4.73553E+01                      4
R259C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.88931E+01    2.62752E-02   -6.81238E-06    8.81463E-10   -4.63099E-14       2
-5.46480E+04   -1.08333E+02   -2.03812E+00    1.22516E-01   -1.14432E-04       3
 5.04665E-08   -7.31290E-12   -4.69070E+04    4.81890E+01                      4
R260C6H12OOOOOH         C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84535E+01    2.78928E-02   -7.55476E-06    1.01448E-09   -5.49949E-14       2
-5.76143E+04   -1.10138E+02   -2.15689E+00    1.14087E-01   -8.63595E-05       3
 2.17195E-08    2.45414E-12   -4.95110E+04    4.69900E+01                      4
R261C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.76572E+01    2.85864E-02   -7.78927E-06    1.05129E-09   -5.72310E-14       2
-4.86688E+04   -9.96720E+01    6.96677E+00    7.24180E-02   -1.22620E-05       3
-3.81540E-08    2.05905E-11   -4.27314E+04    9.56388E+00                      4
R262C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.80950E+01    2.84406E-02   -7.77012E-06    1.04949E-09   -5.70945E-14       2
-4.52514E+04   -1.01696E+02    7.35346E+00    6.88038E-02   -7.26991E-07       3
-5.06200E-08    2.50466E-11   -3.91425E+04    8.64423E+00                      4
R263C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.76572E+01    2.85864E-02   -7.78927E-06    1.05129E-09   -5.72310E-14       2
-4.86688E+04   -9.96720E+01    6.96677E+00    7.24180E-02   -1.22620E-05       3
-3.81540E-08    2.05905E-11   -4.27314E+04    9.56388E+00                      4
R264C4H8OHOO            C   4H   9O   3     G  0300.00   5000.00  1000.00      1
 1.81363E+01    1.91239E-02   -5.13295E-06    6.84034E-10   -3.68440E-14       2
-3.72496E+04   -6.37197E+01    4.03151E+00    4.41240E-02    3.43342E-06       3
-3.52505E-08    1.64927E-11   -3.28225E+04    1.22754E+01                      4
R265C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.85589E+01    2.63225E-02   -6.79623E-06    8.77186E-10   -4.60340E-14       2
-5.53767E+04   -1.07812E+02   -2.50728E+00    1.26811E-01   -1.26995E-04       3
 6.34498E-08   -1.18243E-11   -4.77762E+04    4.84828E+01                      4
R266C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92913E+01    2.61976E-02   -6.83236E-06    8.89020E-10   -4.69549E-14       2
-5.12143E+04   -1.11522E+02   -1.67207E+00    1.19056E-01   -1.03293E-04       3
 3.84188E-08   -3.01181E-12   -4.33160E+04    4.59691E+01                      4
R267C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.82550E+01    2.68924E-02   -7.06534E-06    9.30354E-10   -4.98887E-14       2
-5.53019E+04   -1.05123E+02   -1.53147E+00    1.19878E-01   -1.11475E-04       3
 4.92758E-08   -7.15539E-12   -4.78703E+04    4.55152E+01                      4
R268C6H12OOOOOH         C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R269C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.88931E+01    2.62752E-02   -6.81238E-06    8.81463E-10   -4.63099E-14       2
-5.46480E+04   -1.09432E+02   -2.03812E+00    1.22516E-01   -1.14432E-04       3
 5.04665E-08   -7.31290E-12   -4.69070E+04    4.70905E+01                      4
R270C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.76572E+01    2.85864E-02   -7.78927E-06    1.05129E-09   -5.72310E-14       2
-4.86688E+04   -9.96720E+01    6.96677E+00    7.24180E-02   -1.22620E-05       3
-3.81540E-08    2.05905E-11   -4.27314E+04    9.56388E+00                      4
R271C6H12OOOOOH         C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84889E+01    2.78279E-02   -7.51552E-06    1.00496E-09   -5.41961E-14       2
-5.73766E+04   -1.11433E+02   -2.12770E+00    1.13897E-01   -8.59333E-05       3
 2.13193E-08    2.58827E-12   -4.92627E+04    4.57660E+01                      4
R272C3H5O4H2            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.87592E+01    1.18685E-02   -2.60912E-06    2.96552E-10   -1.41140E-14       2
-2.12813E+04   -5.95781E+01    2.79513E+00    6.52872E-02   -7.36435E-05       3
 4.50951E-08   -1.12080E-11   -1.73093E+04    2.06618E+01                      4
R273C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13660E+01    1.66180E-02   -3.97960E-06    4.83042E-10   -2.41241E-14       2
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-2.49689E+04   -7.15394E+01    1.72784E+00    8.33471E-02   -9.45224E-05       3
 5.90079E-08   -1.50802E-11   -2.01343E+04    2.69143E+01                      4
R274C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.11676E+01    1.69970E-02   -4.13553E-06    5.09939E-10   -2.58693E-14       2
-2.49358E+04   -7.05352E+01    2.85042E+00    7.54180E-02   -7.66630E-05       3
 4.25471E-08   -9.61697E-12   -2.02444E+04    2.22234E+01                      4
R275C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.08996E+01    1.65822E-02   -3.92680E-06    4.74628E-10   -2.37472E-14       2
-2.37191E+04   -7.04355E+01    3.89339E+00    5.64367E-02   -1.96339E-05       3
-1.89563E-08    1.23560E-11   -1.90227E+04    1.84204E+01                      4
R276C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.07002E+01    1.69631E-02   -4.08401E-06    5.01978E-10   -2.55415E-14       2
-8.16135E+03   -6.94251E+01    4.88214E+00    4.94282E-02   -3.96693E-06       3
-3.32472E-08    1.70574E-11   -3.59417E+03    1.42974E+01                      4
R277C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.13095E+01    1.64534E-02   -3.90839E-06    4.72547E-10   -2.35914E-14       2
-2.33634E+04   -7.30002E+01    4.17840E+00    5.34911E-02   -9.90598E-06       3
-2.94510E-08    1.60729E-11   -1.84904E+04    1.72485E+01                      4
R278C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34137E+01    2.26040E-02   -5.91183E-06    7.70978E-10   -4.07926E-14       2
-2.75184E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27012E+04    7.52925E+00                      4
R279C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.51247E+01    2.11684E-02   -5.44625E-06    7.00661E-10   -3.66592E-14       2
-2.80751E+04   -9.03536E+01    1.30674E+00    9.50521E-02   -9.14654E-05       3
 4.51975E-08   -8.58952E-12   -2.19395E+04    3.06072E+01                      4
R280C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75521E+04   -9.10902E+01    4.22835E+00    8.49150E-02   -2.11348E-05       3
-3.50701E-08    2.06357E-11   -3.15840E+04    2.04822E+01                      4
R281C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.52734E+01    3.80893E-02   -1.13921E-05    1.64770E-09   -9.42758E-14       2
-1.07730E+04   -9.00507E+01    5.25056E+00    7.76706E-02   -4.89258E-06       3
-4.99424E-08    2.55448E-11   -4.93759E+03    1.62181E+01                      4
R282C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.58821E+01    3.75773E-02   -1.12142E-05    1.61839E-09   -9.24009E-14       2
-3.71953E+04   -9.36200E+01    4.40669E+00    8.27208E-02   -1.32383E-05       3
-4.37136E-08    2.36904E-11   -3.10404E+04    1.97604E+01                      4
R283C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30628E+01    2.26809E-02   -5.91285E-06    7.70758E-10   -4.08506E-14       2
-2.82411E+04   -7.83263E+01    6.81537E+00    5.94061E-02   -1.84344E-05       3
-1.90940E-08    1.19627E-11   -2.36170E+04    7.06306E+00                      4
R284C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34609E+01    2.25479E-02   -5.88607E-06    7.65681E-10   -4.03913E-14       2
-2.43625E+04   -8.02932E+01    6.77455E+00    5.86963E-02   -1.43078E-05       3
-2.38039E-08    1.35825E-11   -1.95253E+04    7.81866E+00                      4
R285C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.31788E+01    2.30804E-02   -6.13379E-06    8.13790E-10   -4.38279E-14       2
-2.42969E+04   -7.88249E+01    7.84149E+00    5.11541E-02    2.62201E-06       3
-3.93384E-08    1.87188E-11   -1.96295E+04    3.36333E+00                      4
R286C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.38050E+01    2.25393E-02   -5.93950E-06    7.80340E-10   -4.15846E-14       2
-2.39812E+04   -8.24935E+01    7.17465E+00    5.49589E-02   -2.69306E-06       3
-3.61678E-08    1.79564E-11   -1.90054E+04    6.15841E+00                      4
R287C5H10OOOOH         C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.43521E+01    2.27447E-02   -6.09758E-06    8.09454E-10   -4.33485E-14       2
-3.34441E+04   -8.93307E+01    9.67386E-01    8.90932E-02   -7.21982E-05       3
 2.62090E-08   -2.32611E-12   -2.70935E+04    3.10109E+01                      4
R288C5H10OOOOH         C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30299E+01    2.41261E-02   -6.59966E-06    8.90840E-10   -4.83656E-14       2
-3.07596E+04   -8.21557E+01    6.73136E+00    4.97118E-02    1.48873E-05       3
-5.34954E-08    2.36395E-11   -2.55572E+04    6.30846E+00                      4
R289C5H10OOH           C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.79790E+01    2.36145E-02   -6.49289E-06    8.81882E-10   -4.82076E-14       2
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-1.71916E+04   -5.88004E+01    5.77216E+00    4.37225E-02    6.60286E-06       3
-3.69192E-08    1.68589E-11   -1.33351E+04    7.23923E+00                      4
R290C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.28017E+01    1.58660E-02   -3.81061E-06    4.64505E-10   -2.33225E-14       2
-2.44501E+04   -7.98594E+01    1.35515E+00    8.42023E-02   -8.67205E-05       3
 4.60256E-08   -9.57270E-12   -1.90155E+04    2.86070E+01                      4
R291C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.32307E+01    2.18569E-02   -5.53991E-06    7.05525E-10   -3.66887E-14       2
-2.73440E+04   -8.09664E+01    3.80998E+00    6.75261E-02   -2.49606E-05       3
-1.91831E-08    1.31163E-11   -2.19428E+04    2.05695E+01                      4
R292C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.32307E+01    2.18569E-02   -5.53991E-06    7.05525E-10   -3.66887E-14       2
-2.73440E+04   -8.09664E+01    3.80998E+00    6.75261E-02   -2.49606E-05       3
-1.91831E-08    1.31163E-11   -2.19428E+04    2.05695E+01                      4
R293C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30448E+01    2.22163E-02   -5.68518E-06    7.29552E-10   -3.81637E-14       2
-2.73168E+04   -8.00338E+01    5.01610E+00    5.90186E-02   -5.71337E-06       3
-3.70287E-08    1.90697E-11   -2.20619E+04    1.55247E+01                      4
R294C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.35591E+01    2.18769E-02   -5.61084E-06    7.24637E-10   -3.82729E-14       2
-2.69569E+04   -8.30806E+01    4.33396E+00    6.29300E-02   -1.12855E-05       3
-3.36009E-08    1.82160E-11   -2.14362E+04    1.83846E+01                      4
R295C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34137E+01    2.26040E-02   -5.91183E-06    7.70978E-10   -4.07926E-14       2
-2.75184E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27012E+04    7.52925E+00                      4
R296C3H5O4H2            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.85938E+01    1.15034E-02   -2.44990E-06    2.71927E-10   -1.27329E-14       2
-2.02105E+04   -6.02783E+01    2.34223E+00    5.60746E-02   -3.97539E-05       3
 6.18067E-09    3.11385E-12   -1.59123E+04    2.33135E+01                      4
R297C3H5O4H2            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.91034E+01    1.11754E-02   -2.38254E-06    2.67780E-10   -1.28299E-14       2
-7.37252E+03   -6.32994E+01    1.55027E+00    6.07582E-02   -4.72050E-05       3
 1.15045E-08    1.58319E-12   -2.79842E+03    2.66369E+01                      4
R298C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.52734E+01    3.80893E-02   -1.13921E-05    1.64770E-09   -9.42758E-14       2
-3.75186E+04   -9.00507E+01    5.25056E+00    7.76706E-02   -4.89258E-06       3
-4.99424E-08    2.55448E-11   -3.16832E+04    1.62181E+01                      4
R299C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.58821E+01    3.75773E-02   -1.12142E-05    1.61839E-09   -9.24009E-14       2
-1.10031E+04   -9.36200E+01    4.40669E+00    8.27208E-02   -1.32383E-05       3
-4.37136E-08    2.36904E-11   -4.84829E+03    1.97604E+01                      4
R300C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75521E+04   -9.10902E+01    4.22835E+00    8.49150E-02   -2.11348E-05       3
-3.50701E-08    2.06357E-11   -3.15840E+04    2.04822E+01                      4
R301C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75521E+04   -9.10902E+01    4.22835E+00    8.49150E-02   -2.11348E-05       3
-3.50701E-08    2.06357E-11   -3.15840E+04    2.04822E+01                      4
R302C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.52734E+01    3.80893E-02   -1.13921E-05    1.64770E-09   -9.42758E-14       2
-3.75186E+04   -9.00507E+01    5.25056E+00    7.76706E-02   -4.89258E-06       3
-4.99424E-08    2.55448E-11   -3.16832E+04    1.62181E+01                      4
R303C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.58821E+01    3.75773E-02   -1.12142E-05    1.61839E-09   -9.24009E-14       2
-3.71953E+04   -9.36200E+01    4.40669E+00    8.27208E-02   -1.32383E-05       3
-4.37136E-08    2.36904E-11   -3.10404E+04    1.97604E+01                      4
R304C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.67462E+01    1.72950E-02   -4.46202E-06    5.76145E-10   -3.02766E-14       2
-1.00666E+04   -5.43474E+01    9.20577E-01    6.50158E-02   -6.06391E-05       3
 3.16774E-08   -6.83465E-12   -5.79011E+03    2.66741E+01                      4
R305C4H9                C   4H   9O   0     G  0300.00   5000.00  1000.00      1
 7.73125E+00    2.37880E-02   -7.32194E-06    1.07963E-09   -6.25284E-14       2
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 4.66958E+03   -1.28601E+01    2.59734E-01    4.63002E-02   -3.08637E-05       3
 1.04408E-08   -9.04074E-13    6.56028E+03    2.51000E+01                      4
R306C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34958E+01    2.24855E-02   -5.84920E-06    7.56928E-10   -3.96704E-14       2
-2.43763E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95190E+04    8.06816E+00                      4
R307C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.30628E+01    2.26809E-02   -5.91285E-06    7.70758E-10   -4.08506E-14       2
-2.82411E+04   -7.83263E+01    6.81537E+00    5.94061E-02   -1.84344E-05       3
-1.90940E-08    1.19627E-11   -2.36170E+04    7.06306E+00                      4
R308C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.31788E+01    2.30804E-02   -6.13379E-06    8.13790E-10   -4.38279E-14       2
-2.42969E+04   -7.88249E+01    7.84149E+00    5.11541E-02    2.62201E-06       3
-3.93384E-08    1.87188E-11   -1.96295E+04    3.36333E+00                      4
R309C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.38050E+01    2.25393E-02   -5.93950E-06    7.80340E-10   -4.15846E-14       2
-2.39812E+04   -8.24935E+01    7.17465E+00    5.49589E-02   -2.69306E-06       3
-3.61678E-08    1.79564E-11   -1.90054E+04    6.15841E+00                      4
R310C5H11              C   5H  11O   0     G  0300.00   5000.00  1000.00      1
 7.22626E+00    3.36165E-02   -1.10815E-05    1.72020E-09   -1.03503E-13       2
 2.27844E+03   -8.15961E+00   -6.61971E-01    6.31951E-02   -4.86146E-05       3
 2.06999E-08   -3.22505E-12    3.76782E+03    2.99721E+01                      4
R311C5H10OOOOH         C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.43521E+01    2.27447E-02   -6.09758E-06    8.09454E-10   -4.33485E-14       2
-3.34441E+04   -9.00238E+01    9.67386E-01    8.90932E-02   -7.21982E-05       3
 2.62090E-08   -2.32611E-12   -2.70935E+04    3.03178E+01                      4
R312C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.11339E+04   -1.02024E+02    7.12280E+00    7.63821E-02   -1.16257E-05       3
-3.82570E-08    2.00314E-11   -2.48587E+04    9.96241E+00                      4
R313C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R314C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77659E+01    3.38078E-02   -9.56073E-06    1.32764E-09   -7.38260E-14       2
-3.14852E+04   -9.94089E+01    6.97507E+00    7.83602E-02   -1.89959E-05       3
-3.01437E-08    1.71654E-11   -2.54054E+04    1.05552E+01                      4
R315C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78572E+01    3.36449E-02   -9.46464E-06    1.30479E-09   -7.19397E-14       2
-3.15214E+04   -9.99164E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R316C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.78572E+01    3.36449E-02   -9.46464E-06    1.30479E-09   -7.19397E-14       2
-3.15214E+04   -9.99164E+01    6.84693E+00    7.92522E-02   -2.11441E-05       3
-2.79964E-08    1.64051E-11   -2.53918E+04    1.10974E+01                      4
R317C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.51329E+01    2.11549E-02   -5.43892E-06    6.99076E-10   -3.65402E-14       2
-2.66693E+04   -9.03990E+01    1.22617E+00    9.56264E-02   -9.28842E-05       3
 4.66514E-08   -9.11622E-12   -2.05221E+04    3.09462E+01                      4
R318C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.51247E+01    2.11684E-02   -5.44625E-06    7.00661E-10   -3.66592E-14       2
-2.80751E+04   -9.03536E+01    1.30674E+00    9.50521E-02   -9.14654E-05       3
 4.51975E-08   -8.58952E-12   -2.19395E+04    3.06072E+01                      4
R319C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34137E+01    2.26040E-02   -5.91183E-06    7.70978E-10   -4.07926E-14       2
-2.75184E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27012E+04    7.52925E+00                      4
R320C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.59368E+01    3.74805E-02   -1.11576E-05    1.60508E-09   -9.13126E-14       2
-3.73184E+04   -9.39268E+01    4.66844E+00    8.09014E-02   -8.86140E-06       3
-4.80859E-08    2.52381E-11   -3.11690E+04    1.86525E+01                      4
R321C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.55086E+01    3.76326E-02   -1.11857E-05    1.61014E-09   -9.17965E-14       2
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-3.75641E+04   -9.12539E+01    4.36718E+00    8.39519E-02   -1.88235E-05       3
-3.73730E-08    2.14488E-11   -3.15988E+04    1.98943E+01                      4
R322C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75521E+04   -9.10902E+01    4.22835E+00    8.49150E-02   -2.11348E-05       3
-3.50701E-08    2.06357E-11   -3.15840E+04    2.04822E+01                      4
R323C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75521E+04   -9.10902E+01    4.22835E+00    8.49150E-02   -2.11348E-05       3
-3.50701E-08    2.06357E-11   -3.15840E+04    2.04822E+01                      4
R324C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.52734E+01    3.80893E-02   -1.13921E-05    1.64770E-09   -9.42758E-14       2
-3.75186E+04   -9.00507E+01    5.25056E+00    7.76706E-02   -4.89258E-06       3
-4.99424E-08    2.55448E-11   -3.16832E+04    1.62181E+01                      4
R325C3H7                C   3H   7O   0     G  0300.00   5000.00  1000.00      1
 3.18504E+00    2.19241E-02   -7.11417E-06    1.09179E-09   -6.51561E-14       2
 9.45590E+03    9.26810E+00    1.12279E+00    2.81622E-02   -7.69315E-06       3
-7.36009E-09    4.81993E-12    9.72805E+03    1.91611E+01                      4
R326C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.25431E+04   -1.02025E+02    7.21867E+00    7.57093E-02   -9.99194E-06       3
-3.99029E-08    2.06183E-11   -2.62778E+04    9.55753E+00                      4
R327C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77519E+01    3.35893E-02   -9.42966E-06    1.29943E-09   -7.17043E-14       2
-2.95367E+04   -9.92811E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28176E+04    2.76165E+01                      4
R328C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77519E+01    3.35893E-02   -9.42966E-06    1.29943E-09   -7.17043E-14       2
-2.95367E+04   -9.92811E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28176E+04    2.76165E+01                      4
R329C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77519E+01    3.35893E-02   -9.42966E-06    1.29943E-09   -7.17043E-14       2
-2.95367E+04   -9.99742E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28176E+04    2.69234E+01                      4
R330C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.38027E+01    2.25445E-02   -5.94320E-06    7.81340E-10   -4.16751E-14       2
-2.53895E+04   -8.24814E+01    7.12280E+00    5.53265E-02   -3.59437E-06       3
-3.52523E-08    1.76277E-11   -2.04090E+04    6.37688E+00                      4
R331C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77301E+01    3.27509E-02   -8.99031E-06    1.21551E-09   -6.60021E-14       2
-3.45407E+04   -1.01155E+02    3.96992E+00    8.74735E-02   -3.03322E-05       3
-2.48408E-08    1.64584E-11   -2.78187E+04    2.34775E+01                      4
R332C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77301E+01    3.27509E-02   -8.99031E-06    1.21551E-09   -6.60021E-14       2
-1.15340E+04   -1.01155E+02    3.96992E+00    8.74735E-02   -3.03322E-05       3
-2.48408E-08    1.64584E-11   -4.81199E+03    2.34775E+01                      4
R333C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77431E+01    3.27279E-02   -8.97683E-06    1.21234E-09   -6.57425E-14       2
-3.45459E+04   -1.01227E+02    3.96233E+00    8.75251E-02   -3.04537E-05       3
-2.47215E-08    1.64168E-11   -2.78178E+04    2.35098E+01                      4
R334C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77431E+01    3.27279E-02   -8.97683E-06    1.21234E-09   -6.57425E-14       2
-3.45459E+04   -1.01227E+02    3.96233E+00    8.75251E-02   -3.04537E-05       3
-2.47215E-08    1.64168E-11   -2.78178E+04    2.35098E+01                      4
R335C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.32375E+01    2.26762E-02   -5.95211E-06    7.82965E-10   -4.19388E-14       2
-2.55053E+04   -7.90064E+01    2.94642E+00    8.40879E-02   -7.73407E-05       3
 3.94239E-08   -8.40356E-12   -2.01118E+04    2.46521E+01                      4
R336C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34958E+01    2.24855E-02   -5.84920E-06    7.56928E-10   -3.96704E-14       2
-2.43763E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95190E+04    8.06816E+00                      4
R337C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.34958E+01    2.24855E-02   -5.84920E-06    7.56928E-10   -3.96704E-14       2
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-2.43763E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95190E+04    8.06816E+00                      4
R338C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.33367E+01    2.25273E-02   -5.87179E-06    7.64747E-10   -4.04749E-14       2
-2.23705E+04   -7.95531E+01    3.02378E+00    8.35852E-02   -7.59269E-05       3
 3.78415E-08   -7.80083E-12   -1.69519E+04    2.43147E+01                      4
R339C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.33367E+01    2.25273E-02   -5.87179E-06    7.64747E-10   -4.04749E-14       2
-2.23705E+04   -8.02462E+01    3.02378E+00    8.35852E-02   -7.59269E-05       3
 3.78415E-08   -7.80083E-12   -1.69519E+04    2.36216E+01                      4
R340C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.43521E+01    2.27447E-02   -6.09758E-06    8.09454E-10   -4.33485E-14       2
-3.34442E+04   -8.93321E+01    9.89811E-01    8.89371E-02   -7.18225E-05       3
 2.58338E-08   -2.19341E-12   -2.70959E+04    3.09148E+01                      4
R341C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.07004E+01    1.73907E-02   -4.26265E-06    5.29194E-10   -2.70132E-14       2
-2.16583E+04   -6.91089E+01    2.96955E+00    7.20411E-02   -6.97457E-05       3
 3.74100E-08   -8.32324E-12   -1.69859E+04    2.12430E+01                      4
R342C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.68898E+01    2.10004E-02   -5.22256E-06    6.55040E-10   -3.36587E-14       2
-4.57118E+04   -1.00043E+02    1.35147E-01    9.98724E-02   -8.50487E-05       3
 3.03017E-08   -1.95522E-12   -3.88118E+04    3.64104E+01                      4
R343C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.68706E+01    2.10357E-02   -5.24388E-06    6.60169E-10   -3.40852E-14       2
-4.96801E+04   -1.00631E+02    2.35528E-01    9.91720E-02   -8.33545E-05       3
 2.85974E-08   -1.34751E-12   -4.27979E+04    3.52927E+01                      4
R344C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.19912E+01    1.67284E-02   -4.11405E-06    5.12458E-10   -2.62442E-14       2
-2.29307E+04   -7.67757E+01    5.88369E+00    5.35289E-02   -1.82088E-05       3
-1.71627E-08    1.11175E-11   -1.83351E+04    7.84390E+00                      4
R345C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.15778E+01    1.68345E-02   -4.11138E-06    5.08825E-10   -2.59040E-14       2
-2.63588E+04   -7.48902E+01    5.66217E+00    5.59936E-02   -2.69755E-05       3
-7.46451E-09    7.64168E-12   -2.19416E+04    8.06466E+00                      4
R346C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.68796E+01    1.72132E-02   -4.43778E-06    5.72297E-10   -3.00242E-14       2
-9.97837E+03   -5.57410E+01    3.67056E-01    6.55525E-02   -5.91959E-05       3
 2.98204E-08   -6.34422E-12   -5.43201E+03    2.91923E+01                      4
R347C4H9                C   4H   9O   0     G  0300.00   5000.00  1000.00      1
 8.37564E+00    2.33434E-02   -7.18929E-06    1.06000E-09   -6.13594E-14       2
 3.95693E+03   -1.81633E+01   -1.27500E+00    5.39217E-02   -4.19539E-05       3
 1.75003E-08   -2.65793E-12    6.31588E+03    3.04740E+01                      4
R348C5H9OO4H2           C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R349C4H7OO4H2           C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.31050E+01    1.85018E-02   -4.70824E-06    6.03006E-10   -3.15750E-14       2
-3.90372E+04   -8.20170E+01    6.12527E+00    5.24386E-02   -4.75401E-06       3
-3.31526E-08    1.68657E-11   -3.39512E+04    8.38840E+00                      4
R350C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92643E+01    2.62471E-02   -6.86229E-06    8.96283E-10   -4.75644E-14       2
-5.09517E+04   -1.10678E+02   -1.91685E+00    1.20757E-01   -1.07386E-04       3
 4.25109E-08   -4.46159E-12   -4.30383E+04    4.76983E+01                      4
R351C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.86548E+01    2.67305E-02   -7.01546E-06    9.19242E-10   -4.89152E-14       2
-5.43487E+04   -1.08497E+02   -8.42443E-01    1.14080E-01   -9.53560E-05       3
 3.27951E-08   -1.42266E-12   -4.67733E+04    4.18025E+01                      4
R352C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92446E+01    2.62814E-02   -6.88196E-06    9.00857E-10   -4.79354E-14       2
-5.08430E+04   -1.11953E+02   -1.87746E+00    1.20474E-01   -1.06684E-04       3
 4.17921E-08   -4.20235E-12   -4.29417E+04    4.61468E+01                      4
R353C4H7OHOOH           C   4H   9O   3     G  0300.00   5000.00  1000.00      1
 1.89413E+01    1.74943E-02   -4.45234E-06    5.68394E-10   -2.95900E-14       2
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-3.05858E+04   -6.42304E+01    4.30180E+00    5.05804E-02   -1.70731E-05       3
-1.49848E-08    9.76482E-12   -2.63530E+04    1.28558E+01                      4
R354C4H8OH              C   4H   9O   1     G  0300.00   5000.00  1000.00      1
 1.46717E+01    1.72340E-02   -4.55739E-06    6.00598E-10   -3.20933E-14       2
-2.14602E+04   -4.99969E+01   -6.07983E-01    6.11723E-02   -5.19334E-05       3
 2.34049E-08   -4.10393E-12   -1.72443E+04    2.87177E+01                      4
R355C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R356C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R357C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.88931E+01    2.62752E-02   -6.81238E-06    8.81463E-10   -4.63099E-14       2
-5.41448E+04   -1.10125E+02   -2.03812E+00    1.22516E-01   -1.14432E-04       3
 5.04665E-08   -7.31290E-12   -4.64038E+04    4.63975E+01                      4
R358C6H11OO4H2          C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.92913E+01    2.61976E-02   -6.83236E-06    8.89020E-10   -4.69549E-14       2
-5.07111E+04   -1.12215E+02   -1.67207E+00    1.19056E-01   -1.03293E-04       3
 3.84188E-08   -3.01181E-12   -4.28128E+04    4.52760E+01                      4
R359C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.04939E+01    1.67318E-02   -3.96453E-06    4.81967E-10   -2.43586E-14       2
-2.75946E+04   -6.84260E+01    3.52913E+00    5.99555E-02   -3.05055E-05       3
-7.51733E-09    8.35623E-12   -2.30710E+04    1.93804E+01                      4
R360C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.45461E+01    2.16238E-02   -5.58976E-06    7.22122E-10   -3.79221E-14       2
-2.70008E+04   -8.69505E+01    2.21088E+00    8.96078E-02   -8.22315E-05       3
 3.81369E-08   -6.45791E-12   -2.11800E+04    2.68063E+01                      4
R361C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.17338E+01    2.60035E-02   -7.34472E-06    1.01417E-09   -5.59045E-14       2
-3.02286E+04   -7.53591E+01    4.56794E+00    6.05514E-02   -2.54493E-06       3
-4.33513E-08    2.22163E-11   -2.52997E+04    1.54913E+01                      4
R362C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.46515E+01    2.14099E-02   -5.53101E-06    7.18853E-10   -3.81737E-14       2
-2.69961E+04   -8.81277E+01    8.88244E-01    9.89192E-02   -1.03395E-04       3
 5.78785E-08   -1.30759E-11   -2.10484E+04    3.16519E+01                      4
R363C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.41463E+01    2.17596E-02   -5.61813E-06    7.27479E-10   -3.83969E-14       2
-3.08779E+04   -8.49714E+01    1.75572E+00    9.37524E-02   -9.45938E-05       3
 5.10513E-08   -1.09758E-11   -2.52186E+04    2.81518E+01                      4
R364C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.27857E+01    2.32045E-02   -6.15556E-06    8.17773E-10   -4.42048E-14       2
-2.81769E+04   -7.68845E+01    7.50795E+00    5.44625E-02   -7.75087E-06       3
-2.83911E-08    1.48911E-11   -2.36812E+04    4.19279E+00                      4
R365C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.07722E+01    2.79446E-02   -8.22252E-06    1.17456E-09   -6.65819E-14       2
-3.68357E+04   -7.32990E+01    3.98808E+00    5.62495E-02    1.27706E-05       3
-5.84226E-08    2.71022E-11   -3.17362E+04    1.69133E+01                      4
R366C4H8OOOOH           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.20218E+01    1.74395E-02   -4.45452E-06    5.73159E-10   -3.01707E-14       2
-2.98131E+04   -7.94808E+01    1.09802E+00    7.76655E-02   -6.60467E-05       3
 2.56165E-08   -2.80149E-12   -2.41782E+04    2.79707E+01                      4
R367C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.28499E+01    2.19595E-02   -5.54909E-06    7.06280E-10   -3.67782E-14       2
-3.12294E+04   -7.90957E+01    3.73250E+00    6.90649E-02   -3.10979E-05       3
-1.24488E-08    1.07748E-11   -2.60220E+04    2.03137E+01                      4
R368C3H5O4H2            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.83596E+01    1.13281E-02   -2.36498E-06    2.58936E-10   -1.20279E-14       2
-2.41099E+04   -5.91275E+01    1.03312E+00    6.63010E-02   -6.55796E-05       3
 3.12088E-08   -5.34218E-12   -1.98698E+04    2.82100E+01                      4
R369C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 1.94786E+01    2.05576E-02   -5.62064E-06    7.61678E-10   -4.16485E-14       2
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-2.66255E+04   -6.52289E+01    4.48263E+00    5.06224E-02    1.63739E-08       3
-4.03826E-08    2.04906E-11   -2.23613E+04    1.40582E+01                      4
R370C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.17338E+01    2.60035E-02   -7.34472E-06    1.01417E-09   -5.59045E-14       2
-8.92422E+03   -7.53591E+01    4.56794E+00    6.05514E-02   -2.54493E-06       3
-4.33513E-08    2.22163E-11   -3.99530E+03    1.54913E+01                      4
R371C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.43379E+01    2.13918E-02   -5.46886E-06    7.02747E-10   -3.68806E-14       2
-3.09079E+04   -8.59370E+01    6.25781E-01    1.01744E-01   -1.12632E-04       3
 6.77164E-08   -1.65192E-11   -2.51079E+04    3.28721E+01                      4
R372C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.72845E+01    3.41201E-02   -9.62805E-06    1.33166E-09   -7.36651E-14       2
-3.53779E+04   -9.70818E+01    8.02255E+00    7.19328E-02   -7.13493E-06       3
-4.00558E-08    2.03676E-11   -2.95947E+04    5.60133E+00                      4
R373C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.77754E+01    3.37641E-02   -9.52839E-06    1.31925E-09   -7.31055E-14       2
-3.46641E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85845E+04    1.01360E+01                      4
R374C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.41463E+01    2.17596E-02   -5.61813E-06    7.27479E-10   -3.83969E-14       2
-3.08779E+04   -8.49714E+01    1.75572E+00    9.37524E-02   -9.45938E-05       3
 5.10513E-08   -1.09758E-11   -2.52186E+04    2.81518E+01                      4
R375C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.58821E+01    3.75773E-02   -1.12142E-05    1.61839E-09   -9.24009E-14       2
-3.71953E+04   -9.36200E+01    4.40669E+00    8.27208E-02   -1.32383E-05       3
-4.37136E-08    2.36904E-11   -3.10404E+04    1.97604E+01                      4
R376C3H5O4H2           C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.81054E+01    1.40054E-02   -3.44398E-06    4.24551E-10   -2.13323E-14       2
-2.35070E+04   -6.02984E+01   -1.66210E+00    8.16867E-02   -9.24917E-05       3
 5.32469E-08   -1.17222E-11   -1.87630E+04    3.84113E+01                      4
R377C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 1.95407E+01    2.04460E-02   -5.55465E-06    7.45995E-10   -4.03561E-14       2
-7.83988E+03   -6.55741E+01    4.44549E+00    5.08742E-02   -5.76638E-07       3
-3.97993E-08    2.02862E-11   -3.54706E+03    1.42163E+01                      4
R378C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.76558E+01    3.37326E-02   -9.50661E-06    1.31680E-09   -7.30931E-14       2
-3.26726E+04   -9.87512E+01    2.91224E+00    1.05372E-01   -8.59036E-05       3
 3.69365E-08   -6.17956E-12   -2.59667E+04    2.83836E+01                      4
R379C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.74585E+01    3.32689E-02   -9.23145E-06    1.26193E-09   -6.92778E-14       2
-3.44803E+04   -9.97477E+01    5.11624E+00    7.93626E-02   -1.19959E-05       3
-4.18140E-08    2.21141E-11   -2.79311E+04    1.86886E+01                      4
R380C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.79982E+01    3.28807E-02   -9.12660E-06    1.24975E-09   -6.87947E-14       2
-3.41292E+04   -1.02932E+02    4.09843E+00    8.56240E-02   -2.32612E-05       3
-3.26630E-08    1.92234E-11   -2.72698E+04    2.29668E+01                      4
R381C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
 2.72806E+01    3.29728E-02   -9.06839E-06    1.23291E-09   -6.74967E-14       2
-3.83977E+04   -9.88988E+01    3.75694E+00    8.99359E-02   -3.86506E-05       3
-1.59634E-08    1.33690E-11   -3.18831E+04    2.37978E+01                      4
R382C4H8OOOOH          C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.09064E+01    1.83898E-02   -4.75218E-06    6.15368E-10   -3.24599E-14       2
-2.63304E+04   -7.27616E+01    1.88363E+00    6.94733E-02   -5.21490E-05       3
 1.71674E-08   -1.25214E-12   -2.09445E+04    2.60456E+01                      4
R383C5H9OO4H2          C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 2.61660E+01    2.11129E-02   -5.18025E-06    6.41385E-10   -3.25516E-14       2
-4.98788E+04   -9.73658E+01   -5.20535E-01    1.06379E-01   -1.05741E-04       3
 5.23179E-08   -9.69754E-12   -4.32911E+04    3.71836E+01                      4
R384C4H7O4H2           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.03834E+01    1.71324E-02   -4.11129E-06    5.01893E-10   -2.52884E-14       2
-2.65961E+04   -6.94546E+01    5.01633E+00    4.70988E-02    1.36562E-06       3
-3.83526E-08    1.88621E-11   -2.21018E+04    1.22221E+01                      4
R385C5H9OO4H2          C   5H  11O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
R386C4H7OHOOOOH          C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.30726E+01    1.85127E-02   -4.70259E-06    6.00351E-10   -3.13022E-14       2
-4.82904E+04   -8.11529E+01    5.87788E+00    5.40946E-02   -9.07239E-06       3
-2.85590E-08    1.51696E-11   -4.31804E+04    1.01463E+01                      4
R387C6H11OO4H2           C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.84275E+01    2.65563E-02   -6.93363E-06    9.09711E-10   -4.87082E-14       2
-5.50723E+04   -1.06674E+02   -2.60184E+00    1.27457E-01   -1.28525E-04       3
 6.49588E-08   -1.23529E-11   -4.75143E+04    4.92901E+01                      4
R388C4H7OO4H2            C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.37982E+01    1.69281E-02   -4.07473E-06    5.00004E-10   -2.53680E-14       2
-4.44767E+04   -8.81998E+01    4.39494E-01    8.01300E-02   -5.51285E-05       3
 6.29801E-09    5.40715E-12   -3.82370E+04    3.21906E+01                      4
R389C6H11OO4H2           C   6H  13O   5     G  0300.00   5000.00  1000.00      1
 2.85589E+01    2.63225E-02   -6.79623E-06    8.77186E-10   -4.60340E-14       2
-5.48735E+04   -1.08505E+02   -2.50728E+00    1.26811E-01   -1.26995E-04       3
 6.34498E-08   -1.18243E-11   -4.72730E+04    4.77897E+01                      4
R390C5H9O4H2             C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.10810E+01    2.65943E-02   -7.56929E-06    1.05474E-09   -5.87221E-14       2
-8.67597E+03   -7.15426E+01    5.12668E+00    5.74883E-02    1.00751E-06       3
-4.47794E-08    2.23673E-11   -4.05424E+03    1.31551E+01                      4
R391C5H9O4H2             C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.17338E+01    2.60035E-02   -7.34472E-06    1.01417E-09   -5.59045E-14       2
-3.01280E+04   -7.53591E+01    4.56794E+00    6.05514E-02   -2.54493E-06       3
-4.33513E-08    2.22163E-11   -2.51990E+04    1.54913E+01                      4
R392C5H9O4H2             C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.13119E+01    2.61479E-02   -7.36989E-06    1.01841E-09   -5.62984E-14       2
-3.04775E+04   -7.27234E+01    4.15882E+00    6.43439E-02   -1.42738E-05       3
-3.08897E-08    1.78129E-11   -2.57178E+04    1.71908E+01                      4
R393C4H7O4H2             C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.18462E+01    1.64178E-02   -3.96000E-06    4.86089E-10   -2.46347E-14       2
-2.72624E+04   -7.46057E+01    1.77139E+00    8.31258E-02   -9.03749E-05       3
 5.23949E-08   -1.21385E-11   -2.22911E+04    2.62909E+01                      4
R394C4H8OOOOH            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 1.86987E+01    2.21618E-02   -6.29440E-06    8.74405E-10   -4.85021E-14       2
-3.33033E+04   -6.41755E+01    4.23203E+00    4.40394E-02    2.08031E-05       3
-6.09064E-08    2.73031E-11   -2.88331E+04    1.40858E+01                      4
R395C5H10OOOOH           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.07522E+01    2.79819E-02   -8.24544E-06    1.18018E-09   -6.70560E-14       2
-3.68285E+04   -7.38832E+01    4.24627E+00    5.44571E-02    1.70777E-05       3
-6.27223E-08    2.86236E-11   -3.17638E+04    1.51269E+01                      4
R396C5H9O4H2             C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.10810E+01    2.65943E-02   -7.56929E-06    1.05474E-09   -5.87221E-14       2
-3.04332E+04   -7.15426E+01    5.12668E+00    5.74883E-02    1.00751E-06       3
-4.47794E-08    2.23673E-11   -2.58114E+04    1.31552E+01                      4
R397C3H6OOOOH            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
 1.72759E+01    1.56753E-02   -4.14727E-06    5.46197E-10   -2.91421E-14       2
-3.01601E+04   -5.89553E+01   -1.98923E+00    7.56273E-02   -7.29458E-05       3
 3.39464E-08   -5.33789E-12   -2.52264E+04    3.87648E+01                      4
R398C4H7O4H2             C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.16792E+01    1.68259E-02   -4.11310E-06    5.08419E-10   -2.58052E-14       2
-2.09642E+04   -7.44847E+01    2.35125E+00    7.45573E-02   -6.93509E-05       3
 3.41284E-08   -6.80880E-12   -1.58045E+04    2.44044E+01                      4
R399C4H7O4H2             C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.12490E+01    1.69611E-02   -4.12718E-06    5.08653E-10   -2.57757E-14       2
-2.30773E+04   -7.11202E+01    2.19451E+00    7.65744E-02   -7.70450E-05       3
 4.27577E-08   -9.90658E-12   -1.81095E+04    2.57368E+01                      4
R400C4H8OOOOH            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.08227E+01    1.76855E-02   -4.40430E-06    5.52612E-10   -2.83842E-14       2
-3.13149E+04   -7.49981E+01    3.27871E+00    4.92090E-02    8.87503E-06       3
-4.98557E-08    2.31906E-11   -2.60009E+04    1.90264E+01                      4
R401C4H6OHO4H2           C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.37889E+01    1.70520E-02   -4.12494E-06    5.07451E-10   -2.57556E-14       2
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-4.15941E+04   -8.32563E+01    6.55848E+00    5.77032E-02   -2.27348E-05       3
-1.51257E-08    1.08595E-11   -3.67547E+04    6.91081E+00                      4
R402C4H6OHO4H2          C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.34078E+01    1.71006E-02   -4.08835E-06    4.95656E-10   -2.47333E-14       2
-4.50352E+04   -7.94718E+01    6.32449E+00    6.02521E-02   -3.16971E-05       3
-5.23972E-09    7.31988E-12   -4.03599E+04    9.26388E+00                      4
R403C4H7OHOOOOH         C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.36930E+01    1.70683E-02   -4.14485E-06    5.15299E-10   -2.65725E-14       2
-5.37015E+04   -8.76253E+01    6.86295E-01    7.83828E-02   -5.13329E-05       3
 2.85115E-09    6.53742E-12   -4.75195E+04    3.11590E+01                      4
R404C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 1.89265E+01    2.09660E-02   -5.73635E-06    7.76301E-10   -4.23261E-14       2
-2.68699E+04   -6.19722E+01    5.14911E+00    4.68057E-02    5.39174E-06       3
-4.36390E-08    2.12905E-11   -2.28845E+04    1.12667E+01                      4
R405C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.63522E+01    1.74212E-02   -4.48514E-06    5.80325E-10   -3.06582E-14       2
-1.39464E+04   -5.24021E+01    6.08161E-01    6.81720E-02   -7.06320E-05       3
 4.22312E-08   -1.05184E-11   -9.84400E+03    2.74149E+01                      4
R406C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.82392E+01    2.31192E-02   -6.26633E-06    8.39046E-10   -4.52331E-14       2
-1.72479E+04   -6.08382E+01    4.62608E+00    5.18306E-02   -1.17247E-05       3
-1.99563E-08    1.12071E-11   -1.32227E+04    1.13342E+01                      4
R407C3H6OOH             C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.38952E+01    1.23966E-02   -2.95766E-06    3.60667E-10   -1.82253E-14       2
-1.03159E+04   -4.19656E+01    1.87135E+00    4.87528E-02   -4.64913E-05       3
 2.50715E-08   -5.50182E-12   -7.03995E+03    1.96369E+01                      4
R408C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
 2.15055E+01    1.62892E-02   -3.86616E-06    4.68617E-10   -2.35248E-14       2
-8.48715E+03   -7.48368E+01    3.50207E+00    5.59849E-02   -1.23847E-05       3
-2.88510E-08    1.62052E-11   -3.40793E+03    1.98059E+01                      4
R409C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
 1.64050E+01    1.74273E-02   -4.49832E-06    5.83776E-10   -3.09406E-14       2
-1.20735E+04   -5.35148E+01    1.10111E-01    6.82705E-02   -6.85864E-05       3
 4.01522E-08   -1.00468E-11   -7.72645E+03    2.95619E+01                      4
R410C4H6OHO4H2          C   4H   9O   5     G  0300.00   5000.00  1000.00      1
 2.44709E+01    1.55104E-02   -3.51429E-06    4.08342E-10   -1.97234E-14       2
-4.70321E+04   -8.86922E+01    1.10526E+00    8.37925E-02   -6.92892E-05       3
 2.05403E-08    7.30701E-13   -4.10656E+04    3.04189E+01                      4
R411C4H7OHOOH           C   4H   9O   3     G  0300.00   5000.00  1000.00      1
 1.84594E+01    1.77218E-02   -4.52090E-06    5.81747E-10   -3.06579E-14       2
-3.39867E+04   -6.12710E+01    4.26656E+00    5.17561E-02   -2.27504E-05       3
-8.36417E-09    7.37639E-12   -2.99795E+04    1.29803E+01                      4
.C3H5Y                  C   3H   5O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C4H7Y                  C   4H   7O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COC2H5                 C   3H   5O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H9Y                  C   5H   9O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COC3H7                 C   4H   7O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COC4H9                 C   5H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COC6H13               C   7H  13O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COC5H11               C   6H  11O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOC3H7               C   4H   7O   2     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOC2H5               C   3H   5O   2     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOOC2H5              C   3H   5O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOOC3H7              C   4H   7O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOOC4H9              C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOOC6H13             C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.COOOC5H11             C   6H  11O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C3H5O#4               C   3H   5O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C4H7O#4               C   4H   7O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C4H7O#5               C   4H   7O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H13O#4              C   7H  13O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H13O#5              C   7H  13O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H13O#6              C   7H  13O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H9O#4               C   5H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H9O#5                C   5H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H9O#6                C   5H   9O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC3H5O#4              C   3H   5O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC4H7O#4              C   4H   7O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC4H7O#5              C   4H   7O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H13O#4             C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H13O#5             C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H13O#6             C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H9O#4              C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H9O#5              C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H9O#6              C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C3H4O#4OOH             C   3H   5O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C4H6O#4OOH             C   4H   7O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C4H6O#5OOH             C   4H   7O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H12O#4OOH            C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H12O#5OOH            C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C7H12O#6OOH            C   7H  13O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H8O#4OOH             C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H8O#5OOH             C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.C5H8O#6OOH             C   5H   9O   3     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC3H4O#4OOH           C   3H   5O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC4H6O#4OOH           C   4H   7O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC4H6O#5OOH           C   4H   7O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H12O#4OOH          C   7H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H12O#5OOH          C   7H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC7H12O#6OOH          C   7H  13O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H8O#4OOH           C   5H   9O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H8O#5OOH           C   5H   9O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
.OOC5H8O#6OOH           C   5H   9O   5     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C2H3O#4COOOH            C   3H   4O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C3H5O#4COOOH            C   4H   6O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C3H5O#5COOOH            C   4H   6O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
```

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 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11O#4COOOH           C   7H  12O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11O#5COOOH           C   7H  12O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H11O#6COOOH           C   7H  12O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H7O#4COOOH            C   5H   8O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H7O#5COOOH            C   5H   8O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C4H7O#6COOOH            C   5H   8O   4     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H12O#3                C   6H  12O   1     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C6H10#ZZ2               C   6H  10O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C7H12#ZZ2               C   7H  12O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4
C8H14#ZZ2               C   8H  14O   0     G  0300.00   5000.00  1000.00      1
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       2
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00       3
 0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00                      4


END

REACTIONS

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

!   4-center molecular reaction :
C5H12O=>C4H8Y+CH3OH       2.8E14   0.0  59000.0  ! BROCARD 1983 A * 7
!C5H12O=>C4H8Y+CH3OH       4.0E13   0.0  59000.0  ! BROCARD 1983

C6H14O=>C4H8Y+C2H5OH       1.0E12   0.0  52000.0  ! El KADI 1995

!   unimolecular initiations :
C6H14O=>R4CH3+R1C5H11O    6.8E+17  0.0  81809.5  ! UI 1 KB
C6H14O=>R15C2H5O+R39C4H9    1.7E+16  0.0  82046.1  ! UI 2 KB
C6H14O=>R11C2H5+R43C4H9O    5.2E+15  0.0  79634.7  ! UI 3 KB
C6H14O=>R4CH3+R2C5H11O    6.1E+16  0.0  82072.2  ! UI 4 KB
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R1C5H11O=>R11C2H5+C2H6CO    4.0E+13  0.0  19000.0  ! DE 7 CW
R2C5H11O=>R39C4H9+HCHO    2.0E+13  0.0  22000.0  ! DE 12 CW

C5H12O=>R4CH3+R1C4H9O    6.6E+17  0.0  81783.8  ! UI 1 KB
C5H12O=>R7CH3O+R39C4H9    1.4E+16  0.0  82071.8  ! UI 2 KB
C5H12O=>R4CH3+R2C4H9O    1.1E+16  0.0  77789.8  ! UI 3 KB
R1C4H9O=>R4CH3+C2H6CO    4.0E+13  0.0  19000.0  ! DE 7
R2C4H9O=>R4CH3+C2H6CO    2.0E+13  0.0  15000.0  ! DE 10

C7H16=>R19C3H7+R20C4H9    8.8E+16  0.0  86591.6  ! UI 1 KB
C7H16=>R11C2H5+R36C5H11    7.6E+16  0.0  85570.3  ! UI 2 KB
C7H16=>R4CH3+RC6H13    1.4E+17  0.0  86952.7  ! UI 3 KB
RC6H13=>C2H4Z+R20C4H9    2.0E+13  0.0  28700.0

!   bimolecular initiations :
C7H16+O2=>R3O2H+R21C7H15    2.0E+12  0.0  48000.0  ! BI 1 CN
C7H16+O2=>R3O2H+R22C7H15    4.0E+12  0.0  48000.0  ! BI 2 CN
C7H16+O2=>R3O2H+R23C7H15    4.0E+12  0.0  48000.0  ! BI 3 CN
C7H16+O2=>R3O2H+R24C7H15    2.5E+13  0.0  49000.0  ! BI 4 CN
C5H12O+O2=>R3O2H+R25C5H11O    3.8E+13  0.0  49000.0  ! BI 5 CN
C5H12O+O2=>R3O2H+R26C5H11O    1.3E+13  0.0  44000.0  ! BI 6 CN
C6H14O+O2=>R3O2H+R27C6H13O    3.8E+13  0.0  49000.0  ! BI 7 CN
C6H14O+O2=>R3O2H+R28C6H13O    2.0E+12  0.0  43000.0  ! BI 8 CN
C6H14O+O2=>R3O2H+R29C6H13O    1.3E+13  0.0  49000.0  ! BI 9 CN

!   additions :

!   additions with oxygen:
R19C3H7+O2=R30C3H7OO    2.2E+19  -2.5  0.0  ! ADO 10 CN
R20C4H9+O2=R31C4H9OO    2.2E+19  -2.5  0.0  ! ADO 11 CN
R21C7H15+O2=R32C7H15OO    2.2E+19  -2.5  0.0  ! ADO 12 CN
R22C7H15+O2=R33C7H15OO    2.2E+19  -2.5  0.0  ! ADO 13 CN
R23C7H15+O2=R34C7H15OO    2.2E+19  -2.5  0.0  ! ADO 14 CN
R24C7H15+O2=R35C7H15OO    2.2E+19  -2.5  0.0  ! ADO 15 CN
R25C5H11O+O2=R37C5H11OOO    2.2E+19  -2.5  0.0  ! ADO 16 CN
R26C5H11O+O2=R38C5H11OOO    2.2E+19  -2.5  0.0  ! ADO 17 CN
R27C6H13O+O2=R40C6H13OOO    2.2E+19  -2.5  0.0  ! ADO 18 CN
R28C6H13O+O2=R41C6H13OOO    2.2E+19  -2.5  0.0  ! ADO 19 CN
R29C6H13O+O2=R42C6H13OOO    2.2E+19  -2.5  0.0  ! ADO 20 CN
R36C5H11+O2=R67C5H11OO    2.2E+19  -2.5  0.0  ! ADO 21 CN
R39C4H9+O2=R72C4H9OO    2.2E+19  -2.5  0.0  ! ADO 22 CN
R44C3H6OOH+O2=R80C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 23 CN
R45C3H6OOH+O2=R81C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 24 CN
R46C4H8OOH+O2=R82C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 25 CN
R47C4H8OOH+O2=R83C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 26 CN
R48C4H8OOH+O2=R84C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 27 CN
R49C7H14OOH+O2=R86C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 28 CN
R50C7H14OOH+O2=R87C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 29 CN
R51C7H14OOH+O2=R88C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 30 CN
R52C7H14OOH+O2=R91C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 31 CN
R53C7H14OOH+O2=R92C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 32 CN
R54C7H14OOH+O2=R94C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 33 CN
R55C7H14OOH+O2=R95C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 34 CN
R56C7H14OOH+O2=R97C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 35 CN
R57C7H14OOH+O2=R100C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 36 CN
R58C7H14OOH+O2=R102C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 37 CN
R59C7H14OOH+O2=R104C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 38 CN
R60C7H14OOH+O2=R105C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 39 CN
R61C7H14OOH+O2=R106C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 40 CN
R62C7H14OOH+O2=R109C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 41 CN
R63C7H14OOH+O2=R111C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 42 CN
R64C7H14OOH+O2=R114C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 43 CN
R65C7H14OOH+O2=R115C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 44 CN
R66C7H14OOH+O2=R117C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 45 CN
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R68C5H11+O2=R122C5H11OO    2.2E+19  -2.5  0.0  ! ADO 46 CN
R69C5H10OOOH+O2=R123C5H10OOOOOH    2.2E+19  -2.5  0.0  ! ADO 47 CN
R70C5H10OOOH+O2=R124C5H10OOOOOH    2.2E+19  -2.5  0.0  ! ADO 48 CN
R71C5H10OOOH+O2=R127C5H10OOOOOH    2.2E+19  -2.5  0.0  ! ADO 49 CN
R73C6H12OOOH+O2=R130C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 50 CN
R74C6H12OOOH+O2=R131C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 51 CN
R75C6H12OOOH+O2=R133C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 52 CN
R76C6H12OOOH+O2=R135C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 53 CN
R77C6H12OOOH+O2=R136C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 54 CN
R78C6H12OOOH+O2=R138C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 55 CN
R79C6H12OOOH+O2=R139C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 56 CN
R85C4H8OOH+O2=R156C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 57 CN
R89C7H14OOH+O2=R172C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 58 CN
R90C5H10OOH+O2=R173C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 59 CN
R93C5H10OOH+O2=R185C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 60 CN
R96C3H6OOH+O2=R191C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 61 CN
R98C7H14OOH+O2=R197C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 62 CN
R99C4H8OOH+O2=R147C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 63 CN
R101C5H10OOH+O2=R203C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 64 CN
R103C7H14OOH+O2=R210C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 65 CN
R107C7H14OOH+O2=R217C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 66 CN
R108C3H6OOH+O2=R143C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 67 CN
R110C4H8OOH+O2=R153C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 68 CN
R112C7H14OOH+O2=R225C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 69 CN
R113C7H14OOH+O2=R226C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 70 CN
R116C7H14OOH+O2=R233C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 71 CN
R118C5H10OOH+O2=R237C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 72 CN
R119C5H10OOH+O2=R238C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 73 CN
R120C5H10OOH+O2=R239C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 74 CN
R121C5H10OOH+O2=R240C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 75 CN
R125C5H10OOOH+O2=R247C5H10OOOOOH    2.2E+19  -2.5  0.0  ! ADO 76 CN
R126C4H8OOH+O2=R248C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 77 CN
R128C5H10OOOH+O2=R251C5H10OOOOOH    2.2E+19  -2.5  0.0  ! ADO 78 CN
R129C4H8OOH+O2=R252C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 79 CN
R132C6H12OOOH+O2=R260C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 80 CN
R137C6H12OOOH+O2=R268C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 81 CN
R140C6H12OOOH+O2=R271C6H12OOOOOH    2.2E+19  -2.5  0.0  ! ADO 82 CN
R174C5H10OOH+O2=R287C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 83 CN
R175C5H10OOH+O2=R288C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 84 CN
R205C5H10OOH+O2=R311C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 85 CN
R241C5H10OOH+O2=R340C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 86 CN
R289C5H10OOH+O2=R365C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 87 CN
R304C4H8OOH+O2=R366C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 88 CN
R305C4H9+O2=R198C4H9OO    2.2E+19  -2.5  0.0  ! ADO 89 CN
R310C5H11+O2=R204C5H11OO    2.2E+19  -2.5  0.0  ! ADO 90 CN
R325C3H7+O2=R218C3H7OO    2.2E+19  -2.5  0.0  ! ADO 91 CN
R346C4H8OOH+O2=R382C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 92 CN
R347C4H9+O2=R249C4H9OO    2.2E+19  -2.5  0.0  ! ADO 93 CN
R353C4H7OHOOH+O2=R386C4H7OHOOOOH    2.2E+19  -2.5  0.0  ! ADO 94 CN
R354C4H8OH+O2=R264C4H8OHOO    2.2E+19  -2.5  0.0  ! ADO 95 CN
R405C4H8OOH+O2=R394C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 96 CN
R406C5H10OOH+O2=R395C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 97 CN
R407C3H6OOH+O2=R397C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 98 CN
R409C4H8OOH+O2=R400C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 99 CN
R411C4H7OHOOH+O2=R403C4H7OHOOOOH    2.2E+19  -2.5  0.0  ! ADO 100 CN

!   isomerisations :
R21C7H15=R24C7H15    1.2E+12  0.0  19800.0  ! IS 101 KB
R22C7H15=R23C7H15    4.0E+11  0.0  17300.0  ! IS 102 KB
R22C7H15=R24C7H15    1.0E+11  0.0  14500.0  ! IS 103 KB
R23C7H15=R24C7H15    1.8E+10  0.0  19900.0  ! IS 104 KB
R25C5H11O=R26C5H11O    6.0E+11  0.0  19800.0  ! IS 105 KB
R27C6H13O=R28C6H13O    4.0E+11  0.0  17300.0  ! IS 106 KB
R27C6H13O=R29C6H13O    1.0E+11  0.0  14500.0  ! IS 107 KB
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R30C3H7OO=R44C3H6OOH    2.3E+12  0.0  32500.0  ! IS 108 KB
R30C3H7OO=R45C3H6OOH    6.0E+11  0.0  28500.0  ! IS 109 KB
R31C4H9OO=R46C4H8OOH    2.3E+12  0.0  32500.0  ! IS 110 KB
R31C4H9OO=R47C4H8OOH    4.0E+11  0.0  25500.0  ! IS 111 KB
R31C4H9OO=R48C4H8OOH    1.0E+11  0.0  25000.0  ! IS 112 KB
R32C7H15OO=R49C7H14OOH    4.7E+12  0.0  32500.0  ! IS 113 KB
R32C7H15OO=R50C7H14OOH    8.0E+11  0.0  25500.0  ! IS 114 KB
R32C7H15OO=R51C7H14OOH    2.1E+11  0.0  25000.0  ! IS 115 KB
R33C7H15OO=R52C7H14OOH    2.3E+12  0.0  32500.0  ! IS 116 KB
R33C7H15OO=R53C7H14OOH    6.0E+11  0.0  28500.0  ! IS 117 KB
R33C7H15OO=R54C7H14OOH    2.3E+12  0.0  32500.0  ! IS 118 KB
R33C7H15OO=R55C7H14OOH    4.0E+11  0.0  25500.0  ! IS 119 KB
R33C7H15OO=R56C7H14OOH    6.9E+10  0.0  22000.0  ! IS 120 KB
R33C7H15OO=R57C7H14OOH    1.8E+10  0.0  24010.0  ! IS 121 KB
R34C7H15OO=R58C7H14OOH    3.5E+12  0.0  35500.0  ! IS 122 KB
R34C7H15OO=R59C7H14OOH    2.3E+12  0.0  32500.0  ! IS 123 KB
R34C7H15OO=R60C7H14OOH    4.0E+11  0.0  25500.0  ! IS 124 KB
R34C7H15OO=R61C7H14OOH    6.9E+10  0.0  22000.0  ! IS 125 KB
R34C7H15OO=R62C7H14OOH    1.2E+10  0.0  21010.0  ! IS 126 KB
R35C7H15OO=R63C7H14OOH    2.3E+12  0.0  32500.0  ! IS 127 KB
R35C7H15OO=R64C7H14OOH    4.0E+11  0.0  25500.0  ! IS 128 KB
R35C7H15OO=R65C7H14OOH    6.9E+10  0.0  22000.0  ! IS 129 KB
R35C7H15OO=R66C7H14OOH    1.2E+10  0.0  21010.0  ! IS 130 KB
R36C5H11=R68C5H11    4.0E+11  0.0  17300.0  ! IS 131 KB
R37C5H11OOO=R69C5H10OOOH    1.2E+12  0.0  28500.0  ! IS 132 KB
!R37C5H11OOO=R70C5H10OOOH    1.0E+11  0.0  25000.0  ! IS 133 KB
R37C5H11OOO=R70C5H10OOOH    1.0E+11  0.0  22000.0  ! IS 133 KB  -2kcal

R38C5H11OOO=R71C5H10OOOH    3.1E+11  0.0  25000.0  ! IS 134 KB
R40C6H13OOO=R73C6H12OOOH    1.2E+12  0.0  28500.0  ! IS 135 KB
R40C6H13OOO=R74C6H12OOOH    6.9E+10  0.0  22000.0  ! IS 136 KB
R40C6H13OOO=R75C6H12OOOH    1.8E+10  0.0  24010.0  ! IS 137 KB
R41C6H13OOO=R76C6H12OOOH    3.5E+12  0.0  35500.0  ! IS 138 KB
R41C6H13OOO=R77C6H12OOOH    3.1E+11  0.0  25000.0  ! IS 139 KB
R42C6H13OOO=R78C6H12OOOH    2.3E+12  0.0  32500.0  ! IS 140 KB
R42C6H13OOO=R79C6H12OOOH    5.3E+10  0.0  24010.0  ! IS 141 KB
R48C4H8OOH=R85C4H8OOH    4.0E+11  0.0  17300.0  ! IS 142 KB
R49C7H14OOH=R50C7H14OOH    4.0E+11  0.0  17300.0  ! IS 143 KB
R49C7H14OOH=R51C7H14OOH    1.0E+11  0.0  14500.0  ! IS 144 KB
R50C7H14OOH=R51C7H14OOH    1.8E+10  0.0  19900.0  ! IS 145 KB
R51C7H14OOH=R89C7H14OOH    2.0E+11  0.0  15300.0  ! IS 146 KB
R52C7H14OOH=R55C7H14OOH    4.0E+11  0.0  17300.0  ! IS 147 KB
R52C7H14OOH=R56C7H14OOH    6.9E+10  0.0  12000.0  ! IS 148 KB
R52C7H14OOH=R57C7H14OOH    1.8E+10  0.0  19900.0  ! IS 149 KB
R53C7H14OOH=R54C7H14OOH    4.0E+11  0.0  17300.0  ! IS 150 KB
R53C7H14OOH=R55C7H14OOH    6.9E+10  0.0  12000.0  ! IS 151 KB
R53C7H14OOH=R56C7H14OOH    1.2E+10  0.0  17400.0  ! IS 152 KB
R53C7H14OOH=R57C7H14OOH    3.1E+09  0.0  23400.0  ! IS 153 KB
R54C7H14OOH=R57C7H14OOH    6.0E+11  0.0  19800.0  ! IS 154 KB
R56C7H14OOH=R98C7H14OOH    2.0E+11  0.0  15300.0  ! IS 155 KB
R57C7H14OOH=R98C7H14OOH    3.5E+10  0.0  10000.0  ! IS 156 KB
R58C7H14OOH=R60C7H14OOH    4.0E+11  0.0  17300.0  ! IS 157 KB
R58C7H14OOH=R61C7H14OOH    6.9E+10  0.0  12000.0  ! IS 158 KB
R58C7H14OOH=R62C7H14OOH    1.2E+10  0.0  17400.0  ! IS 159 KB
R58C7H14OOH=R103C7H14OOH    3.1E+09  0.0  23400.0  ! IS 160 KB
R59C7H14OOH=R62C7H14OOH    4.0E+11  0.0  17300.0  ! IS 161 KB
R59C7H14OOH=R103C7H14OOH    1.0E+11  0.0  14500.0  ! IS 162 KB
R60C7H14OOH=R103C7H14OOH    6.0E+11  0.0  19800.0  ! IS 163 KB
R61C7H14OOH=R107C7H14OOH    2.0E+11  0.0  15300.0  ! IS 164 KB
R62C7H14OOH=R107C7H14OOH    3.5E+10  0.0  10000.0  ! IS 165 KB
R63C7H14OOH=R66C7H14OOH    4.0E+11  0.0  17300.0  ! IS 166 KB
R63C7H14OOH=R112C7H14OOH    6.9E+10  0.0  12000.0  ! IS 167 KB
R63C7H14OOH=R113C7H14OOH    1.8E+10  0.0  19900.0  ! IS 168 KB
R64C7H14OOH=R112C7H14OOH    4.0E+11  0.0  17300.0  ! IS 169 KB
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R64C7H14OOH=R113C7H14OOH    1.0E+11  0.0  14500.0  ! IS 170 KB
R65C7H14OOH=R113C7H14OOH    6.0E+11  0.0  19800.0  ! IS 171 KB
R65C7H14OOH=R116C7H14OOH    4.0E+11  0.0  17300.0  ! IS 172 KB
R66C7H14OOH=R116C7H14OOH    6.9E+10  0.0  12000.0  ! IS 173 KB
R67C5H11OO=R118C5H10OOH    2.3E+12  0.0  32500.0  ! IS 174 KB
R67C5H11OO=R119C5H10OOH    4.0E+11  0.0  25500.0  ! IS 175 KB
R67C5H11OO=R120C5H10OOH    6.9E+10  0.0  22000.0  ! IS 176 KB
R67C5H11OO=R121C5H10OOH    1.8E+10  0.0  24010.0  ! IS 177 KB
R69C5H10OOOH=R70C5H10OOOH    6.0E+11  0.0  19800.0  ! IS 178 KB
R70C5H10OOOH=R125C5H10OOOH    4.0E+11  0.0  17300.0  ! IS 179 KB
R71C5H10OOOH=R128C5H10OOOH    4.0E+11  0.0  17300.0  ! IS 180 KB
R72C4H9OO=R129C4H8OOH    1.1E+13  0.0  35500.0  ! IS 181 KB
R73C6H12OOOH=R74C6H12OOOH    4.0E+11  0.0  17300.0  ! IS 182 KB
R73C6H12OOOH=R75C6H12OOOH    1.0E+11  0.0  14500.0  ! IS 183 KB
R74C6H12OOOH=R132C6H12OOOH    4.0E+11  0.0  17300.0  ! IS 184 KB
R75C6H12OOOH=R132C6H12OOOH    6.9E+10  0.0  12000.0  ! IS 185 KB
R76C6H12OOOH=R77C6H12OOOH    3.1E+11  0.0  14500.0  ! IS 186 KB
R77C6H12OOOH=R137C6H12OOOH    2.0E+11  0.0  15300.0  ! IS 187 KB
R78C6H12OOOH=R79C6H12OOOH    1.8E+12  0.0  19800.0  ! IS 188 KB
R79C6H12OOOH=R140C6H12OOOH    6.9E+10  0.0  12000.0  ! IS 189 KB
R80C3H6OOOOH=R141C3H5O4H2    3.5E+12  0.0  35500.0  ! IS 190 KB
R80C3H6OOOOH=R142C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 191 KB
R80C3H6OOOOH=R143C3H6OOOOH    3.5E+10  0.0  25000.0  ! IS 192 KB
R81C3H6OOOOH=R144C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 193 KB
R81C3H6OOOOH=R145C3H5O4H2    4.0E+11  0.0  25500.0  ! IS 194 KB
R82C4H8OOOOH=R146C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 195 KB
R82C4H8OOOOH=R147C4H8OOOOH    3.5E+10  0.0  25000.0  ! IS 196 KB
R82C4H8OOOOH=R148C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 197 KB
R82C4H8OOOOH=R149C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 198 KB
R83C4H8OOOOH=R150C4H7O4H2    3.5E+12  0.0  35500.0  ! IS 199 KB
R83C4H8OOOOH=R151C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 200 KB
R83C4H8OOOOH=R152C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 201 KB
R83C4H8OOOOH=R153C4H8OOOOH    5.9E+09  0.0  24010.0  ! IS 202 KB
R84C4H8OOOOH=R154C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 203 KB
R84C4H8OOOOH=R155C4H7O4H2    6.9E+10  0.0  22000.0  ! IS 204 KB
R86C7H14OOOOH=R157C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 205 KB
R86C7H14OOOOH=R158C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 206 KB
R86C7H14OOOOH=R159C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 207 KB
R86C7H14OOOOH=R94C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 208 KB
R86C7H14OOOOH=R160C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 209 KB
R86C7H14OOOOH=R161C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 210 KB
R86C7H14OOOOH=R162C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 211 KB
R87C7H14OOOOH=R163C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 212 KB
R87C7H14OOOOH=R164C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 213 KB
R87C7H14OOOOH=R165C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 214 KB
R87C7H14OOOOH=R105C7H14OOOOH    5.9E+09  0.0  24010.0  ! IS 215 KB
R87C7H14OOOOH=R166C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 216 KB
R87C7H14OOOOH=R167C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 217 KB
R88C7H14OOOOH=R168C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 218 KB
R88C7H14OOOOH=R169C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 219 KB
R88C7H14OOOOH=R170C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 220 KB
R88C7H14OOOOH=R171C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 221 KB
R122C5H11OO=R90C5H10OOH    3.5E+12  0.0  35500.0  ! IS 222 KB
R90C5H10OOH=R174C5H10OOH    4.0E+11  0.0  17300.0  ! IS 223 KB
R90C5H10OOH=R175C5H10OOH    1.0E+11  0.0  14500.0  ! IS 224 KB
R91C7H14OOOOH=R176C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 225 KB
R91C7H14OOOOH=R177C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 226 KB
R91C7H14OOOOH=R104C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 227 KB
R91C7H14OOOOH=R178C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 228 KB
R91C7H14OOOOH=R179C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 229 KB
R91C7H14OOOOH=R180C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 230 KB
R92C7H14OOOOH=R181C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 231 KB
R92C7H14OOOOH=R182C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 232 KB
R92C7H14OOOOH=R114C7H14OOOOH    5.9E+09  0.0  24010.0  ! IS 233 KB
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R92C7H14OOOOH=R183C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 234 KB
R92C7H14OOOOH=R184C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 235 KB
R93C5H10OOH=R120C5H10OOH    4.0E+11  0.0  17300.0  ! IS 236 KB
R93C5H10OOH=R121C5H10OOH    1.0E+11  0.0  14500.0  ! IS 237 KB
R94C7H14OOOOH=R160C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 238 KB
R94C7H14OOOOH=R161C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 239 KB
R94C7H14OOOOH=R162C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 240 KB
R94C7H14OOOOH=R186C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 241 KB
R94C7H14OOOOH=R157C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 242 KB
R94C7H14OOOOH=R158C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 243 KB
R95C7H14OOOOH=R187C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 244 KB
R95C7H14OOOOH=R188C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 245 KB
R95C7H14OOOOH=R189C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 246 KB
R95C7H14OOOOH=R190C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 247 KB
R97C7H14OOOOH=R192C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 248 KB
R97C7H14OOOOH=R193C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 249 KB
R97C7H14OOOOH=R194C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 250 KB
R97C7H14OOOOH=R195C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 251 KB
R97C7H14OOOOH=R196C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 252 KB
R198C4H9OO=R99C4H8OOH    3.5E+12  0.0  35500.0  ! IS 253 KB
R99C4H8OOH=R110C4H8OOH    6.0E+11  0.0  19800.0  ! IS 254 KB
R100C7H14OOOOH=R199C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 255 KB
R100C7H14OOOOH=R200C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 256 KB
R100C7H14OOOOH=R201C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 257 KB
R100C7H14OOOOH=R202C7H13O4H2    5.9E+09  0.0  18010.0  ! IS 258 KB
R204C5H11OO=R101C5H10OOH    1.2E+12  0.0  28500.0  ! IS 259 KB
R101C5H10OOH=R205C5H10OOH    4.0E+11  0.0  17300.0  ! IS 260 KB
R102C7H14OOOOH=R206C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 261 KB
R102C7H14OOOOH=R111C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 262 KB
R102C7H14OOOOH=R207C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 263 KB
R102C7H14OOOOH=R208C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 264 KB
R102C7H14OOOOH=R209C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 265 KB
R103C7H14OOH=R107C7H14OOH    5.9E+09  0.0  15400.0  ! IS 266 KB
R104C7H14OOOOH=R211C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 267 KB
R104C7H14OOOOH=R176C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 268 KB
R104C7H14OOOOH=R178C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 269 KB
R104C7H14OOOOH=R179C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 270 KB
R104C7H14OOOOH=R180C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 271 KB
R104C7H14OOOOH=R212C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 272 KB
R105C7H14OOOOH=R166C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 273 KB
R105C7H14OOOOH=R167C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 274 KB
R105C7H14OOOOH=R213C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 275 KB
R105C7H14OOOOH=R164C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 276 KB
R105C7H14OOOOH=R214C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 277 KB
R105C7H14OOOOH=R163C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 278 KB
R106C7H14OOOOH=R196C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 279 KB
R106C7H14OOOOH=R215C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 280 KB
R106C7H14OOOOH=R194C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 281 KB
R106C7H14OOOOH=R193C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 282 KB
R106C7H14OOOOH=R216C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 283 KB
R106C7H14OOOOH=R192C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 284 KB
R218C3H7OO=R108C3H6OOH    7.0E+12  0.0  35500.0  ! IS 285 KB
R109C7H14OOOOH=R219C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 286 KB
R109C7H14OOOOH=R220C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 287 KB
R109C7H14OOOOH=R221C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 288 KB
R109C7H14OOOOH=R222C7H13O4H2    5.9E+09  0.0  18010.0  ! IS 289 KB
R198C4H9OO=R110C4H8OOH    6.0E+11  0.0  28500.0  ! IS 290 KB
R111C7H14OOOOH=R223C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 291 KB
R111C7H14OOOOH=R207C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 292 KB
R111C7H14OOOOH=R208C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 293 KB
R111C7H14OOOOH=R209C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 294 KB
R111C7H14OOOOH=R224C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 295 KB
R112C7H14OOH=R116C7H14OOH    1.2E+10  0.0  17400.0  ! IS 296 KB
R113C7H14OOH=R116C7H14OOH    2.0E+09  0.0  20900.0  ! IS 297 KB
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R114C7H14OOOOH=R181C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 298 KB
R114C7H14OOOOH=R227C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 299 KB
R114C7H14OOOOH=R183C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 300 KB
R114C7H14OOOOH=R184C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 301 KB
R114C7H14OOOOH=R228C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 302 KB
R114C7H14OOOOH=R229C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 303 KB
R115C7H14OOOOH=R171C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 304 KB
R115C7H14OOOOH=R230C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 305 KB
R115C7H14OOOOH=R231C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 306 KB
R115C7H14OOOOH=R169C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 307 KB
R115C7H14OOOOH=R168C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 308 KB
R115C7H14OOOOH=R232C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 309 KB
R117C7H14OOOOH=R234C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 310 KB
R117C7H14OOOOH=R235C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 311 KB
R117C7H14OOOOH=R201C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 312 KB
R117C7H14OOOOH=R200C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 313 KB
R117C7H14OOOOH=R199C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 314 KB
R117C7H14OOOOH=R236C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 315 KB
R118C5H10OOH=R121C5H10OOH    6.0E+11  0.0  19800.0  ! IS 316 KB
R122C5H11OO=R241C5H10OOH    2.3E+12  0.0  32500.0  ! IS 317 KB
R122C5H11OO=R174C5H10OOH    4.0E+11  0.0  25500.0  ! IS 318 KB
R122C5H11OO=R175C5H10OOH    1.0E+11  0.0  25000.0  ! IS 319 KB
R123C5H10OOOOOH=R242C5H9OO4H2    6.0E+11  0.0  28500.0  ! IS 320 KB
R123C5H10OOOOOH=R243C5H9OO4H2    4.0E+11  0.0  25500.0  ! IS 321 KB
!R123C5H10OOOOOH=R244C5H9OO4H2    1.0E+11  0.0  25000.0  ! IS 322 KB
R123C5H10OOOOOH=R244C5H9OO4H2    1.0E+11  0.0  23000.0  ! IS 322 KB   -2kcal

R124C5H10OOOOOH=R245C5H9OO4H2    2.1E+11  0.0  25000.0  ! IS 323 KB
R124C5H10OOOOOH=R246C5H9OO4H2    6.9E+10  0.0  22000.0  ! IS 324 KB
R249C4H9OO=R126C4H8OOH    1.2E+12  0.0  29500.0  ! IS 325 KB
R127C5H10OOOOOH=R245C5H9OO4H2    1.2E+12  0.0  28500.0  ! IS 326 KB
R127C5H10OOOOOH=R250C5H9OO4H2    6.9E+10  0.0  22000.0  ! IS 327 KB
R130C6H12OOOOOH=R253C6H11OO4H2    6.0E+11  0.0  28500.0  ! IS 328 KB
R130C6H12OOOOOH=R254C6H11OO4H2    4.0E+11  0.0  25500.0  ! IS 329 KB
R130C6H12OOOOOH=R255C6H11OO4H2    6.9E+10  0.0  22000.0  ! IS 330 KB
R130C6H12OOOOOH=R256C6H11OO4H2    1.8E+10  0.0  24010.0  ! IS 331 KB
R131C6H12OOOOOH=R257C6H11OO4H2    3.5E+12  0.0  35500.0  ! IS 332 KB
R131C6H12OOOOOH=R258C6H11OO4H2    2.1E+11  0.0  25000.0  ! IS 333 KB
R131C6H12OOOOOH=R259C6H11OO4H2    6.9E+10  0.0  22000.0  ! IS 334 KB
R133C6H12OOOOOH=R261C6H11OO4H2    2.3E+12  0.0  32500.0  ! IS 335 KB
R133C6H12OOOOOH=R262C6H11OO4H2    3.6E+10  0.0  24010.0  ! IS 336 KB
R133C6H12OOOOOH=R263C6H11OO4H2    1.2E+10  0.0  21010.0  ! IS 337 KB
R134C4H8OOOH=R264C4H8OHOO    2.0E+13  0.0  24000.0  ! IS 338 KB
R135C6H12OOOOOH=R265C6H11OO4H2    1.2E+12  0.0  29500.0  ! IS 339 KB
R135C6H12OOOOOH=R138C6H12OOOOOH    3.5E+10  0.0  25000.0  ! IS 340 KB
R135C6H12OOOOOH=R266C6H11OO4H2    5.3E+10  0.0  24010.0  ! IS 341 KB
R136C6H12OOOOOH=R258C6H11OO4H2    1.2E+12  0.0  28500.0  ! IS 342 KB
R136C6H12OOOOOH=R267C6H11OO4H2    3.5E+10  0.0  19000.0  ! IS 343 KB
R136C6H12OOOOOH=R257C6H11OO4H2    1.8E+10  0.0  24010.0  ! IS 344 KB
R138C6H12OOOOOH=R269C6H11OO4H2    2.3E+12  0.0  32500.0  ! IS 345 KB
R138C6H12OOOOOH=R266C6H11OO4H2    3.1E+11  0.0  25000.0  ! IS 346 KB
R139C6H12OOOOOH=R262C6H11OO4H2    1.2E+12  0.0  28500.0  ! IS 347 KB
R139C6H12OOOOOH=R261C6H11OO4H2    6.9E+10  0.0  22000.0  ! IS 348 KB
R139C6H12OOOOOH=R270C6H11OO4H2    1.2E+10  0.0  21010.0  ! IS 349 KB
R143C3H6OOOOH=R141C3H5O4H2    6.0E+11  0.0  28500.0  ! IS 350 KB
R143C3H6OOOOH=R272C3H5O4H2    1.2E+12  0.0  29500.0  ! IS 351 KB
R146C4H7O4H2=R149C4H7O4H2    6.0E+11  0.0  19800.0  ! IS 352 KB
R147C4H8OOOOH=R273C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 353 KB
R147C4H8OOOOH=R148C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 354 KB
R147C4H8OOOOH=R149C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 355 KB
R150C4H7O4H2=R152C4H7O4H2    4.0E+11  0.0  17300.0  ! IS 356 KB
R153C4H8OOOOH=R150C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 357 KB
R153C4H8OOOOH=R151C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 358 KB
R153C4H8OOOOH=R274C4H7O4H2    2.0E+11  0.0  22500.0  ! IS 359 KB
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R156C4H8OOOOH=R275C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 360 KB
R156C4H8OOOOH=R276C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 361 KB
R156C4H8OOOOH=R277C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 362 KB
R157C7H13O4H2=R160C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 363 KB
R157C7H13O4H2=R161C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 364 KB
R157C7H13O4H2=R162C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 365 KB
R158C7H13O4H2=R159C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 366 KB
R158C7H13O4H2=R160C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 367 KB
R158C7H13O4H2=R161C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 368 KB
R158C7H13O4H2=R162C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 369 KB
R159C7H13O4H2=R162C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 370 KB
R161C7H13O4H2=R186C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 371 KB
R162C7H13O4H2=R186C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 372 KB
R163C7H13O4H2=R165C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 373 KB
R163C7H13O4H2=R166C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 374 KB
R163C7H13O4H2=R167C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 375 KB
R163C7H13O4H2=R213C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 376 KB
R164C7H13O4H2=R167C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 377 KB
R164C7H13O4H2=R213C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 378 KB
R165C7H13O4H2=R213C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 379 KB
R166C7H13O4H2=R214C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 380 KB
R167C7H13O4H2=R214C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 381 KB
R168C7H13O4H2=R171C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 382 KB
R168C7H13O4H2=R230C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 383 KB
R168C7H13O4H2=R231C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 384 KB
R169C7H13O4H2=R230C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 385 KB
R169C7H13O4H2=R231C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 386 KB
R170C7H13O4H2=R231C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 387 KB
R170C7H13O4H2=R232C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 388 KB
R171C7H13O4H2=R232C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 389 KB
R172C7H14OOOOH=R280C7H13O4H2    4.7E+12  0.0  32500.0  ! IS 390 KB
R172C7H14OOOOH=R281C7H13O4H2    8.0E+11  0.0  25500.0  ! IS 391 KB
R172C7H14OOOOH=R282C7H13O4H2    2.1E+11  0.0  25000.0  ! IS 392 KB
R173C5H10OOOOH=R283C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 393 KB
R173C5H10OOOOH=R237C5H10OOOOH    3.5E+10  0.0  25000.0  ! IS 394 KB
R173C5H10OOOOH=R284C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 395 KB
R173C5H10OOOOH=R285C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 396 KB
R173C5H10OOOOH=R286C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 397 KB
R175C5H10OOH=R289C5H10OOH    2.0E+11  0.0  15300.0  ! IS 398 KB
R176C7H13O4H2=R178C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 399 KB
R176C7H13O4H2=R179C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 400 KB
R176C7H13O4H2=R180C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 401 KB
R176C7H13O4H2=R212C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 402 KB
R177C7H13O4H2=R180C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 403 KB
R177C7H13O4H2=R212C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 404 KB
R178C7H13O4H2=R212C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 405 KB
R179C7H13O4H2=R211C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 406 KB
R180C7H13O4H2=R211C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 407 KB
R181C7H13O4H2=R184C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 408 KB
R181C7H13O4H2=R228C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 409 KB
R181C7H13O4H2=R229C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 410 KB
R182C7H13O4H2=R228C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 411 KB
R182C7H13O4H2=R229C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 412 KB
R183C7H13O4H2=R229C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 413 KB
R183C7H13O4H2=R227C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 414 KB
R184C7H13O4H2=R227C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 415 KB
R185C5H10OOOOH=R291C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 416 KB
R185C5H10OOOOH=R292C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 417 KB
R185C5H10OOOOH=R293C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 418 KB
R185C5H10OOOOH=R294C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 419 KB
R187C7H13O4H2=R190C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 420 KB
R187C7H13O4H2=R188C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 421 KB
R188C7H13O4H2=R189C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 422 KB
R188C7H13O4H2=R190C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 423 KB
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R191C3H6OOOOH=R296C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 424 KB
R191C3H6OOOOH=R297C3H5O4H2    6.0E+11  0.0  28500.0  ! IS 425 KB
R192C7H13O4H2=R194C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 426 KB
R192C7H13O4H2=R195C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 427 KB
R192C7H13O4H2=R196C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 428 KB
R192C7H13O4H2=R215C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 429 KB
R193C7H13O4H2=R196C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 430 KB
R193C7H13O4H2=R215C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 431 KB
R194C7H13O4H2=R215C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 432 KB
R195C7H13O4H2=R216C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 433 KB
R196C7H13O4H2=R216C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 434 KB
R197C7H14OOOOH=R298C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 435 KB
R197C7H14OOOOH=R299C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 436 KB
R197C7H14OOOOH=R300C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 437 KB
R197C7H14OOOOH=R301C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 438 KB
R197C7H14OOOOH=R302C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 439 KB
R197C7H14OOOOH=R303C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 440 KB
R198C4H9OO=R304C4H8OOH    2.3E+12  0.0  32500.0  ! IS 441 KB
R199C7H13O4H2=R202C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 442 KB
R199C7H13O4H2=R234C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 443 KB
R199C7H13O4H2=R235C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 444 KB
R200C7H13O4H2=R234C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 445 KB
R200C7H13O4H2=R235C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 446 KB
R201C7H13O4H2=R235C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 447 KB
R201C7H13O4H2=R236C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 448 KB
R202C7H13O4H2=R236C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 449 KB
R203C5H10OOOOH=R306C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 450 KB
R203C5H10OOOOH=R307C5H9O4H2    2.0E+11  0.0  22500.0  ! IS 451 KB
R203C5H10OOOOH=R238C5H10OOOOH    5.9E+09  0.0  24010.0  ! IS 452 KB
R203C5H10OOOOH=R308C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 453 KB
R203C5H10OOOOH=R309C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 454 KB
R204C5H11OO=R205C5H10OOH    4.7E+12  0.0  32500.0  ! IS 455 KB
R206C7H13O4H2=R209C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 456 KB
R206C7H13O4H2=R224C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 457 KB
R206C7H13O4H2=R312C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 458 KB
R207C7H13O4H2=R224C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 459 KB
R207C7H13O4H2=R312C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 460 KB
R208C7H13O4H2=R312C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 461 KB
R208C7H13O4H2=R223C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 462 KB
R209C7H13O4H2=R223C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 463 KB
R210C7H14OOOOH=R313C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 464 KB
R210C7H14OOOOH=R314C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 465 KB
R210C7H14OOOOH=R315C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 466 KB
R210C7H14OOOOH=R316C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 467 KB
R211C7H13O4H2=R212C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 468 KB
R213C7H13O4H2=R214C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 469 KB
R215C7H13O4H2=R216C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 470 KB
R217C7H14OOOOH=R320C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 471 KB
R217C7H14OOOOH=R321C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 472 KB
R217C7H14OOOOH=R322C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 473 KB
R217C7H14OOOOH=R323C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 474 KB
R217C7H14OOOOH=R324C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 475 KB
R219C7H13O4H2=R221C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 476 KB
R219C7H13O4H2=R220C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 477 KB
R219C7H13O4H2=R222C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 478 KB
R220C7H13O4H2=R222C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 479 KB
R223C7H13O4H2=R224C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 480 KB
R223C7H13O4H2=R312C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 481 KB
R225C7H14OOOOH=R326C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 482 KB
R225C7H14OOOOH=R316C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 483 KB
R225C7H14OOOOH=R315C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 484 KB
R225C7H14OOOOH=R314C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 485 KB
R225C7H14OOOOH=R313C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 486 KB
R226C7H14OOOOH=R327C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 487 KB
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R226C7H14OOOOH=R328C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 488 KB
R226C7H14OOOOH=R329C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 489 KB
R227C7H13O4H2=R228C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 490 KB
R227C7H13O4H2=R229C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 491 KB
R230C7H13O4H2=R232C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 492 KB
R231C7H13O4H2=R232C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 493 KB
R233C7H14OOOOH=R331C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 494 KB
R233C7H14OOOOH=R332C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 495 KB
R233C7H14OOOOH=R333C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 496 KB
R233C7H14OOOOH=R334C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 497 KB
R234C7H13O4H2=R236C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 498 KB
R235C7H13O4H2=R236C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 499 KB
R237C5H10OOOOH=R278C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 500 KB
R237C5H10OOOOH=R284C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 501 KB
R237C5H10OOOOH=R285C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 502 KB
R237C5H10OOOOH=R286C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 503 KB
R238C5H10OOOOH=R308C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 504 KB
R238C5H10OOOOH=R309C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 505 KB
R238C5H10OOOOH=R306C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 506 KB
R238C5H10OOOOH=R295C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 507 KB
R239C5H10OOOOH=R330C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 508 KB
R239C5H10OOOOH=R336C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 509 KB
R239C5H10OOOOH=R337C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 510 KB
R239C5H10OOOOH=R319C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 511 KB
R240C5H10OOOOH=R338C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 512 KB
R240C5H10OOOOH=R339C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 513 KB
R240C5H10OOOOH=R335C5H9O4H2    1.2E+10  0.0  21010.0  ! IS 514 KB
R242C5H9OO4H2=R244C5H9OO4H2    6.0E+11  0.0  19800.0  ! IS 515 KB
R243C5H9OO4H2=R244C5H9OO4H2    6.0E+11  0.0  19800.0  ! IS 516 KB
R245C5H9OO4H2=R250C5H9OO4H2    4.0E+11  0.0  17300.0  ! IS 517 KB
R246C5H9OO4H2=R250C5H9OO4H2    4.0E+11  0.0  17300.0  ! IS 518 KB
R247C5H10OOOOOH=R342C5H9OO4H2    1.2E+12  0.0  28500.0  ! IS 519 KB
R247C5H10OOOOOH=R343C5H9OO4H2    1.0E+11  0.0  25000.0  ! IS 520 KB
R248C4H8OOOOH=R344C4H7O4H2    7.0E+12  0.0  35500.0  ! IS 521 KB
R248C4H8OOOOH=R345C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 522 KB
R248C4H8OOOOH=R252C4H8OOOOH    3.5E+10  0.0  25000.0  ! IS 523 KB
R249C4H9OO=R346C4H8OOH    1.2E+12  0.0  28500.0  ! IS 524 KB
R251C5H10OOOOOH=R348C5H9OO4H2    3.1E+11  0.0  25000.0  ! IS 525 KB
R252C4H8OOOOH=R344C4H7O4H2    1.2E+12  0.0  28500.0  ! IS 526 KB
R253C6H11OO4H2=R255C6H11OO4H2    4.0E+11  0.0  17300.0  ! IS 527 KB
R253C6H11OO4H2=R256C6H11OO4H2    1.0E+11  0.0  14500.0  ! IS 528 KB
R254C6H11OO4H2=R255C6H11OO4H2    4.0E+11  0.0  17300.0  ! IS 529 KB
R254C6H11OO4H2=R256C6H11OO4H2    1.0E+11  0.0  14500.0  ! IS 530 KB
R257C6H11OO4H2=R258C6H11OO4H2    2.1E+11  0.0  14500.0  ! IS 531 KB
R257C6H11OO4H2=R259C6H11OO4H2    6.9E+10  0.0  12000.0  ! IS 532 KB
R258C6H11OO4H2=R267C6H11OO4H2    2.0E+11  0.0  15300.0  ! IS 533 KB
R259C6H11OO4H2=R267C6H11OO4H2    2.0E+11  0.0  15300.0  ! IS 534 KB
R260C6H12OOOOOH=R350C6H11OO4H2    1.2E+12  0.0  28500.0  ! IS 535 KB
R260C6H12OOOOOH=R351C6H11OO4H2    6.9E+10  0.0  22000.0  ! IS 536 KB
R260C6H12OOOOOH=R352C6H11OO4H2    1.8E+10  0.0  24010.0  ! IS 537 KB
R261C6H11OO4H2=R262C6H11OO4H2    1.2E+12  0.0  19800.0  ! IS 538 KB
R261C6H11OO4H2=R263C6H11OO4H2    4.0E+11  0.0  17300.0  ! IS 539 KB
R262C6H11OO4H2=R270C6H11OO4H2    6.9E+10  0.0  12000.0  ! IS 540 KB
R263C6H11OO4H2=R270C6H11OO4H2    6.9E+10  0.0  12000.0  ! IS 541 KB
R264C4H8OHOO=R353C4H7OHOOH    1.2E+12  0.0  28500.0  ! IS 542 KB
R265C6H11OO4H2=R266C6H11OO4H2    1.8E+12  0.0  19800.0  ! IS 543 KB
R266C6H11OO4H2=R269C6H11OO4H2    6.9E+10  0.0  12000.0  ! IS 544 KB
R268C6H12OOOOOH=R355C6H11OO4H2    3.5E+12  0.0  35500.0  ! IS 545 KB
R268C6H12OOOOOH=R356C6H11OO4H2    3.1E+11  0.0  25000.0  ! IS 546 KB
R271C6H12OOOOOH=R357C6H11OO4H2    2.3E+12  0.0  32500.0  ! IS 547 KB
R271C6H12OOOOOH=R358C6H11OO4H2    5.3E+10  0.0  24010.0  ! IS 548 KB
R277C4H7O4H2=R359C4H7O4H2    2.0E+11  0.0  15300.0  ! IS 549 KB
R278C5H9O4H2=R285C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 550 KB
R278C5H9O4H2=R286C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 551 KB
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R311C5H10OOOOH=R279C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 552 KB
R340C5H10OOOOH=R279C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 553 KB
R279C5H9O4H2=R360C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 554 KB
R279C5H9O4H2=R317C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 555 KB
R280C7H13O4H2=R281C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 556 KB
R280C7H13O4H2=R282C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 557 KB
R281C7H13O4H2=R282C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 558 KB
R283C5H9O4H2=R286C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 559 KB
R287C5H10OOOOH=R318C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 560 KB
R287C5H10OOOOH=R362C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 561 KB
R287C5H10OOOOH=R363C5H9O4H2    2.0E+11  0.0  22500.0  ! IS 562 KB
R288C5H10OOOOH=R337C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 563 KB
R288C5H10OOOOH=R336C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 564 KB
R288C5H10OOOOH=R364C5H9O4H2    3.5E+10  0.0  19000.0  ! IS 565 KB
R288C5H10OOOOH=R330C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 566 KB
R366C4H8OOOOH=R290C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 567 KB
R291C5H9O4H2=R294C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 568 KB
R293C5H9O4H2=R367C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 569 KB
R294C5H9O4H2=R367C5H9O4H2    3.5E+10  0.0  10000.0  ! IS 570 KB
R295C5H9O4H2=R308C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 571 KB
R295C5H9O4H2=R309C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 572 KB
R298C7H13O4H2=R301C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 573 KB
R298C7H13O4H2=R302C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 574 KB
R298C7H13O4H2=R303C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 575 KB
R299C7H13O4H2=R300C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 576 KB
R299C7H13O4H2=R301C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 577 KB
R299C7H13O4H2=R302C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 578 KB
R299C7H13O4H2=R303C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 579 KB
R300C7H13O4H2=R303C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 580 KB
R306C5H9O4H2=R309C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 581 KB
R311C5H10OOOOH=R371C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 582 KB
R311C5H10OOOOH=R340C5H10OOOOH    3.5E+10  0.0  25000.0  ! IS 583 KB
R311C5H10OOOOH=R360C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 584 KB
R311C5H10OOOOH=R317C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 585 KB
R313C7H13O4H2=R316C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 586 KB
R313C7H13O4H2=R372C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 587 KB
R313C7H13O4H2=R326C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 588 KB
R314C7H13O4H2=R372C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 589 KB
R314C7H13O4H2=R326C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 590 KB
R315C7H13O4H2=R326C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 591 KB
R315C7H13O4H2=R373C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 592 KB
R316C7H13O4H2=R373C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 593 KB
R340C5H10OOOOH=R317C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 594 KB
R317C5H9O4H2=R374C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 595 KB
R318C5H9O4H2=R363C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 596 KB
R319C5H9O4H2=R364C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 597 KB
R319C5H9O4H2=R330C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 598 KB
R320C7H13O4H2=R322C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 599 KB
R320C7H13O4H2=R323C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 600 KB
R320C7H13O4H2=R324C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 601 KB
R320C7H13O4H2=R375C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 602 KB
R321C7H13O4H2=R324C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 603 KB
R321C7H13O4H2=R375C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 604 KB
R322C7H13O4H2=R375C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 605 KB
R326C7H13O4H2=R373C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 606 KB
R327C7H13O4H2=R328C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 607 KB
R327C7H13O4H2=R378C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 608 KB
R328C7H13O4H2=R378C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 609 KB
R329C7H13O4H2=R378C7H13O4H2    8.0E+11  0.0  17300.0  ! IS 610 KB
R330C5H9O4H2=R337C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 611 KB
R331C7H13O4H2=R334C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 612 KB
R331C7H13O4H2=R379C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 613 KB
R331C7H13O4H2=R380C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 614 KB
R332C7H13O4H2=R379C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 615 KB
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R332C7H13O4H2=R380C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 616 KB
R333C7H13O4H2=R380C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 617 KB
R333C7H13O4H2=R381C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 618 KB
R334C7H13O4H2=R381C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 619 KB
R335C5H9O4H2=R338C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 620 KB
R340C5H10OOOOH=R360C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 621 KB
R340C5H10OOOOH=R374C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 622 KB
R382C4H8OOOOH=R341C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 623 KB
R342C5H9OO4H2=R343C5H9OO4H2    6.0E+11  0.0  19800.0  ! IS 624 KB
R343C5H9OO4H2=R383C5H9OO4H2    2.0E+11  0.0  15300.0  ! IS 625 KB
R348C5H9OO4H2=R385C5H9OO4H2    2.0E+11  0.0  15300.0  ! IS 626 KB
R349C4H7OO4H2=R386C4H7OHOOOOH    2.0E+13  0.0  24000.0  ! IS 627 KB
R350C6H11OO4H2=R351C6H11OO4H2    4.0E+11  0.0  17300.0  ! IS 628 KB
R350C6H11OO4H2=R352C6H11OO4H2    1.0E+11  0.0  14500.0  ! IS 629 KB
R351C6H11OO4H2=R387C6H11OO4H2    2.0E+11  0.0  15300.0  ! IS 630 KB
R352C6H11OO4H2=R387C6H11OO4H2    3.5E+10  0.0  10000.0  ! IS 631 KB
R355C6H11OO4H2=R356C6H11OO4H2    3.1E+11  0.0  14500.0  ! IS 632 KB
R357C6H11OO4H2=R358C6H11OO4H2    1.8E+12  0.0  19800.0  ! IS 633 KB
R358C6H11OO4H2=R389C6H11OO4H2    3.5E+10  0.0  10000.0  ! IS 634 KB
R365C5H10OOOOH=R361C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 635 KB
R361C5H9O4H2=R390C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 636 KB
R361C5H9O4H2=R391C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 637 KB
R365C5H10OOOOH=R392C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 638 KB
R365C5H10OOOOH=R390C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 639 KB
R365C5H10OOOOH=R391C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 640 KB
R366C4H8OOOOH=R393C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 641 KB
R394C4H8OOOOH=R369C4H7O4H2    3.5E+12  0.0  35500.0  ! IS 642 KB
R369C4H7O4H2=R377C4H7O4H2    6.0E+11  0.0  19800.0  ! IS 643 KB
R395C5H10OOOOH=R370C5H9O4H2    1.2E+12  0.0  28500.0  ! IS 644 KB
R370C5H9O4H2=R396C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 645 KB
R372C7H13O4H2=R373C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 646 KB
R397C3H6OOOOH=R376C3H5O4H2    7.0E+12  0.0  35500.0  ! IS 647 KB
R394C4H8OOOOH=R377C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 648 KB
R379C7H13O4H2=R381C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 649 KB
R380C7H13O4H2=R381C7H13O4H2    1.0E+09  0.0  18900.0  ! IS 650 KB
R382C4H8OOOOH=R398C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 651 KB
R382C4H8OOOOH=R399C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 652 KB
R400C4H8OOOOH=R384C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 653 KB
R386C4H7OHOOOOH=R401C4H6OHO4H2    6.0E+11  0.0  28500.0  ! IS 654 KB
R386C4H7OHOOOOH=R402C4H6OHO4H2    4.0E+11  0.0  25500.0  ! IS 655 KB
R388C4H7OO4H2=R403C4H7OHOOOOH    2.0E+13  0.0  24000.0  ! IS 656 KB
R394C4H8OOOOH=R404C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 657 KB
R395C5H10OOOOH=R396C5H9O4H2    4.7E+12  0.0  32500.0  ! IS 658 KB
R400C4H8OOOOH=R408C4H7O4H2    1.2E+12  0.0  28500.0  ! IS 659 KB
R403C4H7OHOOOOH=R410C4H6OHO4H2    1.2E+12  0.0  28500.0  ! IS 660 KB

!   beta-scissions :
R19C3H7=>R4CH3+C2H4Z    2.0E+13  0.0  31000.0  ! DE 661 CN
R20C4H9=>R11C2H5+C2H4Z    2.0E+13  0.0  28700.0  ! DE 662 CW
R21C7H15=>R11C2H5+C5H10Z    4.0E+13  0.0  28700.0  ! DE 663 CW
R22C7H15=>R19C3H7+C4H8Y    2.0E+13  0.0  28700.0  ! DE 664 CW
R22C7H15=>R4CH3+C6H12Z    2.0E+13  0.0  31000.0  ! DE 665 CN
R23C7H15=>R20C4H9+C3H6Y    2.0E+13  0.0  28700.0  ! DE 666 CW
R24C7H15=>R36C5H11+C2H4Z    2.0E+13  0.0  28700.0  ! DE 667 CW
R25C5H11O=>R7CH3O+C4H8Y    2.0E+13  0.0  26000.0  ! DE 668c
R25C5H11O=>R4CH3+C4H8OY    4.0E+13  0.0  31000.0  ! DE 669 CN
R26C5H11O=>R39C4H9+HCHO    2.0E+13  0.0  24000.0  ! DE 670 CWc
R27C6H13O=>R15C2H5O+C4H8Y    2.0E+13  0.0  24000.0  ! DE 671
R27C6H13O=>R4CH3+C5H10OY    4.0E+13  0.0  31000.0  ! DE 672 CN
R28C6H13O=>R39C4H9+CH3CHO    2.0E+13  0.0  24000.0  ! DE 673 CWc
R29C6H13O=>R43C4H9O+C2H4Z    2.0E+13  0.0  26000.0  ! DE 674c
R36C5H11=>R19C3H7+C2H4Z    2.0E+13  0.0  28700.0  ! DE 675 CW
R43C4H9O=>R4CH3+C2H6CO    4.0E+13  0.0  15300.0  ! DE 676
R44C3H6OOH=>R3O2H+C3H6Y    8.5E+12  0.0  26000.0  ! DE 677 CR
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R46C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 678 CR
R46C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 679 CN
R48C4H8OOH=>R16C2H4O2H+C2H4Z    2.0E+13  0.0  28700.0  ! DE 680 CW
R49C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 681 CN
R49C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 682 CR
R49C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 683 CW
R50C7H14OOH=>R85C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 684 CW
R51C7H14OOH=>R90C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 685 CW
R52C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 686 CW
R52C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 687 CR
R53C7H14OOH=>R93C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 688 CW
R54C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 689 CR
R54C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 690 CW
     DUPLICATE
R54C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 691 CW
     DUPLICATE
R55C7H14OOH=>R96C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 692 CW
R55C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 693 CN
R56C7H14OOH=>R99C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 694 CW
R57C7H14OOH=>R101C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 695 CW
R58C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 696 CR
R59C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 697 CN
R59C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 698 CR
R59C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 699 CW
R60C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 700 CW
R61C7H14OOH=>R108C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 701 CW
R61C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 702 CN
R62C7H14OOH=>R110C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 703 CW
R63C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 704 CW
R63C7H14OOH=>R3O2H+C7H14Z    8.5E+12  0.0  26000.0  ! DE 705 CR
R64C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 706 CW
R65C7H14OOH=>R16C2H4O2H+C5H10Z    2.0E+13  0.0  28700.0  ! DE 707 CW
R65C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 708 CW
R66C7H14OOH=>R45C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 709 CW
R66C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 710 CN
R68C5H11=>R11C2H5+C3H6Y    2.0E+13  0.0  28700.0  ! DE 711 CW
R69C5H10OOOH=>R7CH3O+C4H7OOHY    2.0E+13  0.0  26000.0  ! DE 712 c
R69C5H10OOOH=>R4CH3+C4H7OOOHY    2.0E+13  0.0  31000.0  ! DE 713 CN
R70C5H10OOOH=>R126C4H8OOH+HCHO    2.0E+13  0.0  24000.0  ! DE 714 CWc
R71C5H10OOOH=>R4CH3+C4H7OOOHY    4.0E+13  0.0  31000.0  ! DE 715 CN
R73C6H12OOOH=>R15C2H5O+C4H7OOHY    2.0E+13  0.0  26000.0  ! DE 716c
R73C6H12OOOH=>R4CH3+C5H9OOOHY    2.0E+13  0.0  31000.0  ! DE 717 CN
R74C6H12OOOH=>R126C4H8OOH+CH3CHO    2.0E+13  0.0  24000.0  ! DE 718 CWc
R75C6H12OOOH=>R134C4H8OOOH+C2H4Z    4.0E+13  0.0  15300.0  ! DE 719
R76C6H12OOOH=>R3O2H+C6H12OZ    8.5E+12  0.0  26000.0  ! DE 720 CR
R77C6H12OOOH=>R4CH3+C5H9OOOHY    4.0E+13  0.0  31000.0  ! DE 721 CN
R78C6H12OOOH=>R3O2H+C6H12OZ    8.5E+12  0.0  26000.0  ! DE 722 CR
R79C6H12OOOH=>R4CH3+C5H9OOOHY    4.0E+13  0.0  31000.0  ! DE 723 CN
R85C4H8OOH=>R2OH+C3H7CHO    1.0E+09  0.0  7500.0  ! DE 724 CW
R89C7H14OOH=>R11C2H5+C5H9OOHZ    4.0E+13  0.0  28700.0  ! DE 725 CW
R89C7H14OOH=>R2OH+C6H14CO    2.0E+09  0.0  7500.0  ! DE 726 CW
R90C5H10OOH=>R3O2H+C5H10Z    8.5E+12  0.0  26000.0  ! DE 727 CR
R93C5H10OOH=>R2OH+C4H9CHO    1.0E+09  0.0  7500.0  ! DE 728 CW
R96C3H6OOH=>R2OH+C2H5CHO    1.0E+09  0.0  7500.0  ! DE 729 CW
R98C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 730 CN
R98C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 731 CW
R98C7H14OOH=>R2OH+C6H14CO    1.0E+09  0.0  7500.0  ! DE 732 CW
R99C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 733 CR
R101C5H10OOH=>R96C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 734 CW
R103C7H14OOH=>R175C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 735 CW
R107C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 736 CW
R107C7H14OOH=>R2OH+C6H14CO    1.0E+09  0.0  7500.0  ! DE 737 CW
R108C3H6OOH=>R3O2H+C3H6Y    8.5E+12  0.0  26000.0  ! DE 738 CR
R112C7H14OOH=>R48C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 739 CW
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R113C7H14OOH=>R121C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 740 CW
R116C7H14OOH=>R2OH+C6H13CHO    1.0E+09  0.0  7500.0  ! DE 741 CW
R118C5H10OOH=>R3O2H+C5H10Z    8.5E+12  0.0  26000.0  ! DE 742 CR
R118C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 743 CW
R119C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 744 CN
R120C5H10OOH=>R16C2H4O2H+C3H6Y    2.0E+13  0.0  28700.0  ! DE 745 CW
R121C5H10OOH=>R45C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 746 CW
R125C5H10OOOH=>R7CH3O+C4H7OOHY    2.0E+13  0.0  26000.0  ! DE 747
R125C5H10OOOH=>R4CH3+C4H7OOOHY    4.0E+13  0.0  31000.0  ! DE 748 CN
R125C5H10OOOH=>R2OH+C4H9OCHO    1.0E+09  0.0  7500.0  ! DE 749 CW
R126C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 750 CR
R128C5H10OOOH=>R2OH+C4H9OCHO    1.0E+09  0.0  7500.0  ! DE 751 CW
R129C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 752 CR
R129C4H8OOH=>R4CH3+C3H5OOHY    4.0E+13  0.0  31000.0  ! DE 753 CN
R132C6H12OOOH=>R15C2H5O+C4H7OOHY    2.0E+13  0.0  26000.0  ! DE 754
R132C6H12OOOH=>R4CH3+C5H9OOOHY    4.0E+13  0.0  31000.0  ! DE 755 CN
R132C6H12OOOH=>R2OH+C5H11OCHO    1.0E+09  0.0  7500.0  ! DE 756 CW
R134C4H8OOOH=>R4CH3+C2H5COOOH    4.0E+13  0.0  15300.0  ! DE 757
R137C6H12OOOH=>R39C4H9+CH3COO2H    2.0E+13  0.0  28700.0  ! DE 758 CW
R137C6H12OOOH=>R2OH+C5H12OCO    1.0E+09  0.0  7500.0  ! DE 759 CW
R140C6H12OOOH=>R2OH+C5H11OCHO    1.0E+09  0.0  7500.0  ! DE 760 CW
R142C3H5O4H2=>R2OH+C2H4CHOOOH    1.0E+09  0.0  7500.0  ! DE 761 CW
R145C3H5O4H2=>R2OH+C2H4CHOOOH    1.0E+09  0.0  7500.0  ! DE 762 CW
R146C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 763 CW
R152C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 764 CW
R155C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 765 CW
R158C7H13O4H2=>R278C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 766 CW
R159C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 767 CW
R162C7H13O4H2=>R279C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 768 CW
R165C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 769 CW
R170C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 770 CW
R175C5H10OOH=>R108C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 771 CW
R177C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 772 CW
R180C7H13O4H2=>R290C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 773 CW
R182C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 774 CW
R186C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 775 CW
R188C7H13O4H2=>R295C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 776 CW
R190C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 777 CW
R195C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 778 CW
R202C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 779 CW
R205C5H10OOH=>R3O2H+C5H10Z    8.5E+12  0.0  26000.0  ! DE 780 CR
R205C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 781 CW
R206C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 782 CW
R211C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 783 CW
R212C7H13O4H2=>R317C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 784 CW
R213C7H13O4H2=>R318C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 785 CW
R214C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 786 CW
R215C7H13O4H2=>R319C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 787 CW
R216C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 788 CW
R222C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 789 CW
R223C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 790 CW
R227C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 791 CW
R231C7H13O4H2=>R330C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 792 CW
R232C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 793 CW
R235C7H13O4H2=>R335C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 794 CW
R236C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 795 CW
R241C5H10OOH=>R3O2H+C5H10Z    8.5E+12  0.0  26000.0  ! DE 796 CR
R241C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 797 CN
     DUPLICATE
R241C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 798 CN
     DUPLICATE
R243C5H9OO4H2=>R2OH+C4H8OCHOOOH    1.0E+09  0.0  7500.0  ! DE 799 CW
R244C5H9OO4H2=>R341C4H7O4H2+HCHO    2.0E+13  0.0  28700.0  ! DE 800 CW
R246C5H9OO4H2=>R2OH+C4H8OCHOOOH    1.0E+09  0.0  7500.0  ! DE 801 CW
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R250C5H9OO4H2=>R2OH+C4H8OCHOOOH    1.0E+09  0.0  7500.0  ! DE 802 CW
R254C6H11OO4H2=>R2OH+C5H10OCHOOOH    1.0E+09  0.0  7500.0  ! DE 803 CW
R256C6H11OO4H2=>R349C4H7OO4H2+C2H4Z    2.0E+13  0.0  24000.0  ! DE 804
R259C6H11OO4H2=>R2OH+C5H10OCHOOOH    1.0E+09  0.0  7500.0  ! DE 805 CW
R263C6H11OO4H2=>R2OH+C5H10OCHOOOH    1.0E+09  0.0  7500.0  ! DE 806 CW
R265C6H11OO4H2=>R2OH+C5H11OCOOOH    1.0E+09  0.0  7500.0  ! DE 807 CW
R267C6H11OO4H2=>R2OH+C5H11OCOOOH    1.0E+09  0.0  7500.0  ! DE 808 CW
R269C6H11OO4H2=>R2OH+C5H10OCHOOOH    1.0E+09  0.0  7500.0  ! DE 809 CW
R270C6H11OO4H2=>R2OH+C5H10OCHOOOH    1.0E+09  0.0  7500.0  ! DE 810 CW
R272C3H5O4H2=>R2OH+C2H5COOOH    1.0E+09  0.0  7500.0  ! DE 811 CW
R273C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 812 CW
R274C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 813 CW
R278C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 814 CW
R282C7H13O4H2=>R361C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 815 CW
R283C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 816 CW
R289C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 817 CW
R289C5H10OOH=>R2OH+C4H10CO    1.0E+09  0.0  7500.0  ! DE 818 CW
R295C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 819 CW
R301C7H13O4H2=>R368C3H5O4H2+C4H8Y    2.0E+13  0.0  28700.0  ! DE 820 CW
R302C7H13O4H2=>R369C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 821 CW
R303C7H13O4H2=>R370C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 822 CW
R304C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 823 CR
R304C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 824 CN
R305C4H9=>R4CH3+C3H6Y    2.0E+13  0.0  31000.0  ! DE 825 CN
R307C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 826 CW
R310C5H11=>R4CH3+C4H8Y    4.0E+13  0.0  31000.0  ! DE 827 CN
R319C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 828 CW
R323C7H13O4H2=>R376C3H5O4H2+C4H8Y    2.0E+13  0.0  28700.0  ! DE 829 CW
R324C7H13O4H2=>R377C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 830 CW
R335C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 831 CW
R343C5H9OO4H2=>R384C4H7O4H2+HCHO    2.0E+13  0.0  28700.0  ! DE 832 CW
R345C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 833 CW
R346C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 834 CN
R347C4H9=>R4CH3+C3H6Y    4.0E+13  0.0  31000.0  ! DE 835 CN
R349C4H7OO4H2=>R4CH3+C2H4COO4H2    4.0E+13  0.0  15300.0  ! DE 836
R352C6H11OO4H2=>R388C4H7OO4H2+C2H4Z    2.0E+13  0.0  24000.0  ! DE 837
R353C4H7OHOOH=>R2OH+C4H7OOHY    2.0E+13  0.0  24000.0  ! DE 838
R353C4H7OHOOH=>R4CH3+C3H4OHOOHZ    2.0E+13  0.0  31000.0  ! DE 839 CN
R354C4H8OH=>R2OH+C4H8Y    2.0E+13  0.0  24000.0  ! DE 840
R354C4H8OH=>R4CH3+C3H5OHY    4.0E+13  0.0  31000.0  ! DE 841 CN
R359C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 842 CW
R363C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 843 CW
R364C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 844 CW
R367C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 845 CW
R368C3H5O4H2=>R2OH+C2H5COOOH    1.0E+09  0.0  7500.0  ! DE 846 CW
R371C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 847 CW
R372C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 848 CW
R373C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 849 CW
R374C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 850 CW
R378C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 851 CW
R381C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 852 CW
R383C5H9OO4H2=>R2OH+C4H9OCOOOH    1.0E+09  0.0  7500.0  ! DE 853 CW
R385C5H9OO4H2=>R2OH+C4H9OCOOOH    1.0E+09  0.0  7500.0  ! DE 854 CW
R387C6H11OO4H2=>R2OH+C5H11OCOOOH    1.0E+09  0.0  7500.0  ! DE 855 CW
R388C4H7OO4H2=>R4CH3+C2H4COO4H2    4.0E+13  0.0  15300.0  ! DE 856
R389C6H11OO4H2=>R2OH+C5H11OCOOOH    1.0E+09  0.0  7500.0  ! DE 857 CW
R393C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 858 CW
R399C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 859 CW
R401C4H6OHO4H2=>R2OH+C4H6O4H2Y    2.0E+13  0.0  24000.0  ! DE 860
R402C4H6OHO4H2=>R2OH+C4H6O4H2Y    2.0E+13  0.0  24000.0  ! DE 861
R402C4H6OHO4H2=>R2OH+C3H5OHCHOOOH    1.0E+09  0.0  7500.0  ! DE 862 CW
R405C4H8OOH=>R2OH+C3H8CO    1.0E+09  0.0  7500.0  ! DE 863 CW
R405C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 864 CN
R406C5H10OOH=>R4CH3+C4H7OOHY    4.0E+13  0.0  31000.0  ! DE 865 CN
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R406C5H10OOH=>R2OH+C4H10CO    2.0E+09  0.0  7500.0  ! DE 866 CW
R407C3H6OOH=>R2OH+C2H6CO    2.0E+09  0.0  7500.0  ! DE 867 CW
R409C4H8OOH=>R4CH3+C3H5OOHY    4.0E+13  0.0  31000.0  ! DE 868 CN
R409C4H8OOH=>R2OH+C3H7CHO    1.0E+09  0.0  7500.0  ! DE 869 CW
R410C4H6OHO4H2=>R2OH+C4H6O4H2Y    2.0E+13  0.0  24000.0  ! DE 870
R411C4H7OHOOH=>R2OH+C4H7OOHY    2.0E+13  0.0  24000.0  ! DE 871
R411C4H7OHOOH=>R4CH3+C3H4OHOOHZ    4.0E+13  0.0  31000.0  ! DE 872 CN
R411C4H7OHOOH=>R2OH+C3H6OHCHO    1.0E+09  0.0  7500.0  ! DE 873 CW

!   decomposition to o-rings :
R44C3H6OOH=>R2OH+C3H6O#3    1.0E+12  0.0  16500.0  ! OR 874 CR
R45C3H6OOH=>R2OH+C3H6O#4    2.0E+11  0.0  15500.0  ! OR 875 CR
R46C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 876 CR
R47C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 877 CR
R48C4H8OOH=>R2OH+C4H8O#5    6.0E+11  0.0  9000.0  ! OR 878 CR
R49C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 879 CR
R50C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 880 CR
R51C7H14OOH=>R2OH+C7H14O#5    6.0E+11  0.0  9000.0  ! OR 881 CR
R52C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 882 CR
R53C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 883 CR
R54C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 884 CR
R55C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 885 CR
R56C7H14OOH=>R2OH+C7H14O#5    6.0E+11  0.0  9000.0  ! OR 886 CR
R57C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 887 CN
R58C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 888 CR
R59C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 889 CR
R60C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 890 CR
R61C7H14OOH=>R2OH+C7H14O#5    6.0E+11  0.0  9000.0  ! OR 891 CR
R62C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 892 CN
R63C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 893 CR
R64C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 894 CR
R65C7H14OOH=>R2OH+C7H14O#5    6.0E+11  0.0  9000.0  ! OR 895 CR
R66C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 896 CN
R69C5H10OOOH=>R2OH+C5H10O2#4    2.0E+11  0.0  15500.0  ! OR 897 CR
R70C5H10OOOH=>R2OH+C5H10O2#4    2.0E+11  0.0  15500.0  ! OR 898 CR
R71C5H10OOOH=>R2OH+C5H10O2#4    2.0E+11  0.0  15500.0  ! OR 899 CR
R73C6H12OOOH=>R2OH+C6H12O2#4    2.0E+11  0.0  15500.0  ! OR 900 CR
R74C6H12OOOH=>R2OH+C6H12O2#4    2.0E+11  0.0  15500.0  ! OR 901 CR
R75C6H12OOOH=>R2OH+C6H12O2#5    6.0E+11  0.0  9000.0  ! OR 902 CR
R76C6H12OOOH=>R2OH+C6H12O2#3    1.0E+12  0.0  16500.0  ! OR 903 CR
R77C6H12OOOH=>R2OH+C6H12O2#4    2.0E+11  0.0  15500.0  ! OR 904 CR
R78C6H12OOOH=>R2OH+C6H12O2#3    1.0E+12  0.0  16500.0  ! OR 905 CR
R79C6H12OOOH=>R2OH+C6H12O2#5    6.0E+11  0.0  9000.0  ! OR 906 CR
R90C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 907 CR
R99C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 908 CR
R101C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 909 CR
R108C3H6OOH=>R2OH+C3H6O#3    1.0E+12  0.0  16500.0  ! OR 910 CR
R110C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 911 CR
R118C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 912 CR
R119C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 913 CR
R120C5H10OOH=>R2OH+C5H10O#5    6.0E+11  0.0  9000.0  ! OR 914 CR
R121C5H10OOH=>R2OH+C5H10O#6    1.0E+10  0.0  6000.0  ! OR 915 CN
R126C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 916 CR
R129C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 917 CR
R141C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 918 CR
R141C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 919 CR
R142C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 920 CR
R144C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 921 CR
R145C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 922 CR
R146C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 923 CR
R148C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 924 CR
R148C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 925 CR
R149C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 926 CR
R149C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+11  0.0  9000.0  ! OR 927 CR
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R150C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 928 CR
R150C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+11  0.0  9000.0  ! OR 929 CR
R151C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 930 CR
     DUPLICATE
R151C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 931 CR
     DUPLICATE
R152C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 932 CR
R154C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 933 CR
R154C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 934 CR
R155C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+11  0.0  9000.0  ! OR 935 CR
R157C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 936 CR
R157C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 937 CR
R158C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 938 CR
R158C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 939 CR
R159C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 940 CR
R160C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 941 CR
R160C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 942 CR
R161C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 943 CR
R161C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 944 CR
R162C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 945 CR
R162C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 946 CN
R163C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 947 CR
R163C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 948 CR
R164C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 949 CR
     DUPLICATE
R164C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 950 CR
     DUPLICATE
R165C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 951 CR
R166C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 952 CR
R166C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 953 CR
R167C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 954 CR
R167C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 955 CN
R168C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 956 CR
R168C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 957 CR
R169C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 958 CR
R169C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 959 CR
R170C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 960 CR
R171C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 961 CR
R171C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 962 CN
R174C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 963 CR
R175C5H10OOH=>R2OH+C5H10O#5    6.0E+11  0.0  9000.0  ! OR 964 CR
R176C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 965 CR
R176C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 966 CR
R177C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 967 CR
R178C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 968 CR
R178C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 969 CR
R179C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 970 CR
R179C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 971 CR
R180C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 972 CR
R180C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 973 CN
R181C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 974 CR
     DUPLICATE
R181C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 975 CR
     DUPLICATE
R182C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 976 CR
R183C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 977 CR
R183C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 978 CR
R184C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 979 CR
R184C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 980 CN
R186C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 981 CR
R187C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 982 CR
R187C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 983 CR
R188C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 984 CR
R188C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 985 CN
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R189C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 986 CR
R190C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 987 CR
R192C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 988 CR
R192C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 989 CN
R193C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 990 CR
R193C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 991 CR
R194C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 992 CR
R194C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 993 CR
R195C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 994 CR
R196C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 995 CR
R196C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 996 CN
R199C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 997 CR
R199C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 998 CR
R200C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 999 CR
     DUPLICATE
R200C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1000 CR
     DUPLICATE
R201C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1001 CR
R201C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1002 CR
R202C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1003 CN
R205C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 1004 CR
R206C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1005 CR
R207C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1006 CR
R207C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1007 CR
R208C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1008 CR
R208C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1009 CR
R209C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1010 CR
R209C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1011 CN
R211C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1012 CR
R212C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1013 CN
R213C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1014 CR
R214C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1015 CR
R215C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1016 CR
R216C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1017 CR
R219C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1018 CR
R220C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1019 CR
R220C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1020 CR
R221C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1021 CR
R222C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1022 CN
R223C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1023 CR
R224C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1024 CN
R227C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1025 CR
R228C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1026 CR
R229C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1027 CN
R230C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1028 CR
R231C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1029 CR
R232C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1030 CR
R234C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1031 CR
R235C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1032 CR
R236C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1033 CN
R241C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 1034 CR
R242C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1035 CR
R243C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1036 CR
R244C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1037 CR
R245C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1038 CR
     DUPLICATE
R245C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1039 CR
     DUPLICATE
R246C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1040 CR
R250C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1041 CR
R253C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1042 CR
R254C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1043 CR
R255C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1044 CR
R256C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1045 CR
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R257C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1046 CR
R257C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1047 CR
R258C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1048 CR
     DUPLICATE
R258C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1049 CR
     DUPLICATE
R259C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1050 CR
R261C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1051 CR
R261C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1052 CR
R262C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1053 CR
R262C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1054 CR
R263C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1055 CR
R265C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1056 CR
R266C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1057 CR
R266C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1058 CR
R267C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1059 CR
R269C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1060 CR
R270C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1061 CR
R272C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1062 CR
R273C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1063 CR
R274C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1064 CR
R275C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1065 CR
R276C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1066 CR
R277C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+11  0.0  9000.0  ! OR 1067 CR
R278C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1068 CR
R279C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1069 CR
R279C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1070 CR
R280C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1071 CR
R281C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1072 CR
R282C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1073 CR
R283C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1074 CR
R284C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1075 CR
R284C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1076 CR
R285C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1077 CR
R285C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1078 CR
R286C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1079 CR
R286C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1080 CN
R290C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1081 CR
R290C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1082 CR
R291C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1083 CR
R292C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1084 CR
R293C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1085 CR
R294C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1086 CN
R295C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1087 CR
R296C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1088 CR
R297C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 1089 CR
R298C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1090 CR
R299C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1091 CR
R300C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1092 CR
R301C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1093 CR
R302C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1094 CR
R303C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1095 CN
R304C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 1096 CR
R306C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1097 CR
     DUPLICATE
R306C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1098 CR
     DUPLICATE
R307C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1099 CR
R308C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1100 CR
R308C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1101 CR
R309C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1102 CR
R309C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1103 CN
R313C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1104 CR
R313C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1105 CN
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R314C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1106 CR
R314C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1107 CR
R315C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1108 CR
R315C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1109 CR
R316C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1110 CR
R316C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1111 CN
R317C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1112 CR
R317C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1113 CR
R318C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1114 CR
R318C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1115 CR
R319C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1116 CR
R320C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1117 CR
R321C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1118 CR
R322C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1119 CR
R323C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1120 CR
R324C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1121 CN
R326C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1122 CR
R327C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1123 CR
R328C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1124 CR
R328C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1125 CN
R329C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1126 CR
R330C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1127 CR
R330C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1128 CN
R331C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1129 CR
R332C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1130 CR
R333C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+11  0.0  9000.0  ! OR 1131 CR
R334C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1132 CN
R335C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1133 CN
R336C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1134 CR
R336C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1135 CR
R337C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1136 CR
R337C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1137 CR
R338C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1138 CR
R338C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1139 CR
R339C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1140 CR
R341C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1141 CR
R342C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1142 CR
R343C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1143 CR
R344C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1144 CR
R344C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1145 CR
R345C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1146 CR
R346C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 1147 CR
R348C5H9OO4H2=>R2OH+C5H9O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1148 CR
R350C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1149 CR
R351C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1150 CR
R352C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1151 CR
R353C4H7OHOOH=>R2OH+C4H8O2#4    2.0E+11  0.0  15500.0  ! OR 1152 CR
R355C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1153 CR
R356C6H11OO4H2=>R2OH+C6H11O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1154 CR
R357C6H11OO4H2=>R2OH+C6H11O2#3OOH    1.0E+12  0.0  16500.0  ! OR 1155 CR
R358C6H11OO4H2=>R2OH+C6H11O2#5OOH    6.0E+11  0.0  9000.0  ! OR 1156 CR
R360C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1157 CR
R360C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1158 CR
R361C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1159 CR
R362C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1160 CR
R363C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1161 CR
R364C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1162 CR
R369C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1163 CR
R370C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1164 CR
R371C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1165 CR
R374C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1166 CR
R376C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1167 CR
R377C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1168 CR
R384C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1169 CR
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R390C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1170 CR
R391C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+11  0.0  9000.0  ! OR 1171 CR
R392C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1172 CR
R393C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1173 CR
R396C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1174 CR
R398C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1175 CR
R399C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1176 CR
R401C4H6OHO4H2=>R2OH+C4H7O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1177 CR
R402C4H6OHO4H2=>R2OH+C4H7O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1178 CR
R404C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1179 CR
R408C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1180 CR
R410C4H6OHO4H2=>R2OH+C4H7O2#4OOH    2.0E+11  0.0  15500.0  ! OR 1181 CR

!   oxidations :
R39C4H9+O2=>C4H8Y+R3O2H    2.1E+12  0.0  5000.0  ! OX 1182 CN
R325C3H7+O2=>C3H6Y+R3O2H    1.4E+12  0.0  5000.0  ! OX 1183 CN
R28C6H13O+O2=>C6H12OZ+R3O2H    6.9E+11  0.0  5000.0  ! OX 378 CN
R29C6H13O+O2=>C6H12OZ+R3O2H    1.6E+12  0.0  5000.0  ! OX 379 CN
R21C7H15+O2=>C7H14Z+R3O2H    3.2E+12  0.0  5000.0  ! OX 1090 CN
R22C7H15+O2=>C7H14Z+R3O2H    3.2E+12  0.0  5000.0  ! OX 1092 CN
R23C7H15+O2=>C7H14Z+R3O2H    2.3E+12  0.0  5000.0  ! OX 1093 CN
R24C7H15+O2=>C7H14Z+R3O2H    1.6E+12  0.0  5000.0  ! OX 1095 CN


!   metathesis :
B1O+C7H16=>R2OH+R21C7H15    2.6E+13  0.0  5200.0  ! ME 1184 CW
B1O+C7H16=>R2OH+R22C7H15    5.2E+13  0.0  5200.0  ! ME 1185 CW
B1O+C7H16=>R2OH+R23C7H15    5.2E+13  0.0  5200.0  ! ME 1186 CW
B1O+C7H16=>R2OH+R24C7H15    1.0E+14  0.0  7850.0  ! ME 1187 CW
B1O+C5H12O=>R2OH+R25C5H11O    1.5E+14  0.0  7850.0  ! ME 1188 CW
B1O+C5H12O=>R2OH+R26C5H11O    5.1E+13  0.0  5850.0  ! ME 1189 CW
B1O+C6H14O=>R2OH+R27C6H13O    1.5E+14  0.0  7850.0  ! ME 1190 CW
B1O+C6H14O=>R2OH+R28C6H13O    2.6E+13  0.0  3200.0  ! ME 1191 CW
B1O+C6H14O=>R2OH+R29C6H13O    5.1E+13  0.0  7850.0  ! ME 1192 CW
C7H16+R1H=>H2+R21C7H15    9.0E+06  2.0  5000.0  ! ME 496 CW
C7H16+R1H=>H2+R22C7H15    1.8E+07  2.0  5000.0  ! ME 497 CW
C7H16+R1H=>H2+R23C7H15    1.8E+07  2.0  5000.0  ! ME 498 CW
C7H16+R1H=>H2+R24C7H15    5.6E+07  2.0  7700.0  ! ME 499 CW
C5H12O+R1H=>H2+R25C5H11O    8.5E+07  2.0  7700.0  ! ME 500 CW
C5H12O+R1H=>H2+R26C5H11O    2.8E+07  2.0  7700.0  ! ME 501 CW
C6H14O+R1H=>H2+R27C6H13O    8.5E+07  2.0  7700.0  ! ME 502 CW
C6H14O+R1H=>H2+R28C6H13O    1.9E+07  2.0  7700.0  ! ME 503 CW
C6H14O+R1H=>H2+R29C6H13O    2.8E+07  2.0  7700.0  ! ME 504 CW
C7H16+R2OH=>H2O+R21C7H15    2.6E+06  2.0  -765.0  ! ME 505 CW
C7H16+R2OH=>H2O+R22C7H15    5.2E+06  2.0  -765.0  ! ME 506 CW
C7H16+R2OH=>H2O+R23C7H15    5.2E+06  2.0  -765.0  ! ME 507 CW
C7H16+R2OH=>H2O+R24C7H15    5.4E+06  2.0  450.0  ! ME 508 CW
C5H12O+R2OH=>H2O+R25C5H11O    8.1E+06  2.0  450.0  ! ME 509 CW
C5H12O+R2OH=>H2O+R26C5H11O    2.7E+06  2.0  450.0  ! ME 510 CW


C6H14O+R2OH=>H2O+R27C6H13O    8.1E+06  2.0  450.0  ! ME 511 CW
C6H14O+R2OH=>H2O+R28C6H13O    2.6E+06  2.0  -765.0  ! ME 512 CW
C6H14O+R2OH=>H2O+R29C6H13O    2.7E+06  2.0  450.0  ! ME 513 CW
C7H16+R3O2H=>H2O2+R21C7H15    4.0E+11  0.0  15500.0  ! ME 514 CN
C7H16+R3O2H=>H2O2+R22C7H15    8.0E+11  0.0  15500.0  ! ME 515 CN
C7H16+R3O2H=>H2O2+R23C7H15    8.0E+11  0.0  15500.0  ! ME 516 CN
C7H16+R3O2H=>H2O2+R24C7H15    1.2E+12  0.0  17000.0  ! ME 517 CN
C5H12O+R3O2H=>H2O2+R25C5H11O    1.8E+12  0.0  17000.0  ! ME 518 CN
C5H12O+R3O2H=>H2O2+R26C5H11O    6.0E+11  0.0  17000.0  ! ME 519 CN

C6H14O+R3O2H=>H2O2+R27C6H13O    1.8E+12  0.0  17000.0  ! ME 520 CN
C6H14O+R3O2H=>H2O2+R28C6H13O    4.0E+11  0.0  15500.0  ! ME 521 CN
C6H14O+R3O2H=>H2O2+R29C6H13O    6.0E+11  0.0  17000.0  ! ME 522 CN
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C7H16+R4CH3=>CH4+R21C7H15    2.0E+11  0.0  9600.0  ! ME 523 CN
C7H16+R4CH3=>CH4+R22C7H15    4.0E+11  0.0  9600.0  ! ME 524 CN
C7H16+R4CH3=>CH4+R23C7H15    4.0E+11  0.0  9600.0  ! ME 525 CN
C7H16+R4CH3=>CH4+R24C7H15    6.0E-01  4.0  8200.0  ! ME 526 CN
C5H12O+R4CH3=>CH4+R25C5H11O    9.0E-01  4.0  8200.0  ! ME 527 CN
C5H12O+R4CH3=>CH4+R26C5H11O    3.0E-01  4.0  8200.0  ! ME 528 CN
C6H14O+R4CH3=>CH4+R27C6H13O    9.0E-01  4.0  8200.0  ! ME 529 CN
C6H14O+R4CH3=>CH4+R28C6H13O    2.0E-01  4.0  8200.0  ! ME 530 CN
C6H14O+R4CH3=>CH4+R29C6H13O    3.0E-01  4.0  8200.0  ! ME 531 CN
C7H16+R5CHO=>HCHO+R21C7H15    1.1E+07  1.9  17000.0  ! ME 532 CN
C7H16+R5CHO=>HCHO+R22C7H15    2.2E+07  1.9  17000.0  ! ME 533 CN
C7H16+R5CHO=>HCHO+R23C7H15    2.2E+07  1.9  17000.0  ! ME 534 CN
C7H16+R5CHO=>HCHO+R24C7H15    2.0E+05  2.5  18500.0  ! ME 535 CN
C5H12O+R5CHO=>HCHO+R25C5H11O    3.1E+05  2.5  18500.0  ! ME 536 CN
C5H12O+R5CHO=>HCHO+R26C5H11O    1.0E+05  2.5  18500.0  ! ME 537 CN
C6H14O+R5CHO=>HCHO+R27C6H13O    3.1E+05  2.5  18500.0  ! ME 538 CN
C6H14O+R5CHO=>HCHO+R28C6H13O    6.8E+04  2.5  18500.0  ! ME 539 CN
C6H14O+R5CHO=>HCHO+R29C6H13O    1.0E+05  2.5  18500.0  ! ME 540 CN
C7H16+R6CH2OH=>CH3OH+R21C7H15    6.0E+01  3.0  12000.0  ! ME 541 CN
C7H16+R6CH2OH=>CH3OH+R22C7H15    1.2E+02  3.0  12000.0  ! ME 542 CN
C7H16+R6CH2OH=>CH3OH+R23C7H15    1.2E+02  3.0  12000.0  ! ME 543 CN
C7H16+R6CH2OH=>CH3OH+R24C7H15    2.0E+02  3.0  14000.0  ! ME 544 CN
C5H12O+R6CH2OH=>CH3OH+R25C5H11O    3.0E+02  3.0  14000.0  ! ME 545 CN
C5H12O+R6CH2OH=>CH3OH+R26C5H11O    9.9E+01  3.0  14000.0  ! ME 546 CN
C6H14O+R6CH2OH=>CH3OH+R27C6H13O    3.0E+02  3.0  14000.0  ! ME 547 CN
C6H14O+R6CH2OH=>CH3OH+R28C6H13O    6.6E+01  3.0  14000.0  ! ME 548 CN
C6H14O+R6CH2OH=>CH3OH+R29C6H13O    9.9E+01  3.0  14000.0  ! ME 549 CN
C7H16+R7CH3O=>CH3OH+R21C7H15    1.5E+11  0.0  4500.0  ! ME 550 CN
C7H16+R7CH3O=>CH3OH+R22C7H15    2.9E+11  0.0  4500.0  ! ME 551 CN
C7H16+R7CH3O=>CH3OH+R23C7H15    2.9E+11  0.0  4500.0  ! ME 552 CN
C7H16+R7CH3O=>CH3OH+R24C7H15    3.2E+11  0.0  7300.0  ! ME 553 CN
C5H12O+R7CH3O=>CH3OH+R25C5H11O    4.9E+11  0.0  7300.0  ! ME 554 CN
C5H12O+R7CH3O=>CH3OH+R26C5H11O    1.6E+11  0.0  7300.0  ! ME 555 CN
C6H14O+R7CH3O=>CH3OH+R27C6H13O    4.9E+11  0.0  7300.0  ! ME 556 CN
C6H14O+R7CH3O=>CH3OH+R28C6H13O    1.1E+11  0.0  7300.0  ! ME 557 CN
C6H14O+R7CH3O=>CH3OH+R29C6H13O    1.6E+11  0.0  7300.0  ! ME 558 CN
C7H16+R8CH3OO=>CH3O2H+R21C7H15    3.0E+12  0.0  17500.0  ! ME 559 CN
C7H16+R8CH3OO=>CH3O2H+R22C7H15    6.0E+12  0.0  17500.0  ! ME 560 CN
C7H16+R8CH3OO=>CH3O2H+R23C7H15    6.0E+12  0.0  17500.0  ! ME 561 CN
C7H16+R8CH3OO=>CH3O2H+R24C7H15    1.2E+13  0.0  20000.0  ! ME 562 CN
C5H12O+R8CH3OO=>CH3O2H+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 563 CN
C5H12O+R8CH3OO=>CH3O2H+R26C5H11O    6.0E+12  0.0  20000.0  ! ME 564 CN
C6H14O+R8CH3OO=>CH3O2H+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 565 CN
C6H14O+R8CH3OO=>CH3O2H+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 566 CN
C6H14O+R8CH3OO=>CH3O2H+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 567 CN
C7H16+R11C2H5=>C2H6+R21C7H15    2.0E+11  0.0  11000.0  ! ME 568 CN
C7H16+R11C2H5=>C2H6+R22C7H15    4.0E+11  0.0  11000.0  ! ME 569 CN
C7H16+R11C2H5=>C2H6+R23C7H15    4.0E+11  0.0  11000.0  ! ME 570 CN
C7H16+R11C2H5=>C2H6+R24C7H15    6.0E+11  0.0  13500.0  ! ME 571 CR
C5H12O+R11C2H5=>C2H6+R25C5H11O    9.0E+11  0.0  13500.0  ! ME 572 CR
C5H12O+R11C2H5=>C2H6+R26C5H11O    3.0E+11  0.0  13500.0  ! ME 573 CR
C6H14O+R11C2H5=>C2H6+R27C6H13O    9.0E+11  0.0  13500.0  ! ME 574 CR
C6H14O+R11C2H5=>C2H6+R28C6H13O    2.0E+11  0.0  13500.0  ! ME 575 CR
C6H14O+R11C2H5=>C2H6+R29C6H13O    3.0E+11  0.0  13500.0  ! ME 576 CR
C7H16+R32C7H15OO=>C7H15OOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 577 CN
C7H16+R32C7H15OO=>C7H15OOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 578 CN
C7H16+R32C7H15OO=>C7H15OOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 579 CN
C7H16+R32C7H15OO=>C7H15OOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 580 CN
C5H12O+R32C7H15OO=>C7H15OOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 581 CN
C5H12O+R32C7H15OO=>C7H15OOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 582 CN  -2
C6H14O+R32C7H15OO=>C7H15OOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 583 CN
C6H14O+R32C7H15OO=>C7H15OOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 584 CN
C6H14O+R32C7H15OO=>C7H15OOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 585 CN
C7H16+R33C7H15OO=>C7H15OOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 586 CN
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C7H16+R33C7H15OO=>C7H15OOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 587 CN
C7H16+R33C7H15OO=>C7H15OOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 588 CN
C7H16+R33C7H15OO=>C7H15OOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 589 CN
C5H12O+R33C7H15OO=>C7H15OOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 590 CN
C5H12O+R33C7H15OO=>C7H15OOH+R26C5H11O    6.0E+12  0.0  20000.0  ! ME 591 CN
C6H14O+R33C7H15OO=>C7H15OOH+R27C6H13O    1.8E+13  0.0  18000.0  ! ME 592 CN  -2
C6H14O+R33C7H15OO=>C7H15OOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 593 CN
C6H14O+R33C7H15OO=>C7H15OOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 594 CN
C7H16+R34C7H15OO=>C7H15OOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 595 CN
C7H16+R34C7H15OO=>C7H15OOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 596 CN
C7H16+R34C7H15OO=>C7H15OOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 597 CN
C7H16+R34C7H15OO=>C7H15OOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 598 CN
C5H12O+R34C7H15OO=>C7H15OOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 599 CN
C5H12O+R34C7H15OO=>C7H15OOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 600 CN   -2
C6H14O+R34C7H15OO=>C7H15OOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 601 CN
C6H14O+R34C7H15OO=>C7H15OOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 602 CN
C6H14O+R34C7H15OO=>C7H15OOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 603 CN
C7H16+R35C7H15OO=>C7H15OOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 604 CN
C7H16+R35C7H15OO=>C7H15OOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 605 CN
C7H16+R35C7H15OO=>C7H15OOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 606 CN
C7H16+R35C7H15OO=>C7H15OOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 607 CN
C5H12O+R35C7H15OO=>C7H15OOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 608 CN
C5H12O+R35C7H15OO=>C7H15OOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 609 CN    -2
C6H14O+R35C7H15OO=>C7H15OOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 610 CN
C6H14O+R35C7H15OO=>C7H15OOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 611 CN
C6H14O+R35C7H15OO=>C7H15OOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 612 CN
C7H16+R38C5H11OOO=>C5H11OOOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 613 CN
C7H16+R38C5H11OOO=>C5H11OOOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 614 CN
C7H16+R38C5H11OOO=>C5H11OOOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 615 CN
C7H16+R38C5H11OOO=>C5H11OOOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 616 CN
C5H12O+R38C5H11OOO=>C5H11OOOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 617 CN
C5H12O+R38C5H11OOO=>C5H11OOOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 618 CN    -2
C6H14O+R38C5H11OOO=>C5H11OOOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 619 CN
C6H14O+R38C5H11OOO=>C5H11OOOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 620 CN
C6H14O+R38C5H11OOO=>C5H11OOOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 621 CN
C7H16+R37C5H11OOO=>C5H11OOOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 622 CN
C7H16+R37C5H11OOO=>C5H11OOOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 623 CN
C7H16+R37C5H11OOO=>C5H11OOOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 624 CN
C7H16+R37C5H11OOO=>C5H11OOOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 625 CN
C5H12O+R37C5H11OOO=>C5H11OOOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 626 CN
C5H12O+R37C5H11OOO=>C5H11OOOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 627 CN    -2
C6H14O+R37C5H11OOO=>C5H11OOOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 628 CN
C6H14O+R37C5H11OOO=>C5H11OOOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 629 CN
C6H14O+R37C5H11OOO=>C5H11OOOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 630 CN
C7H16+R40C6H13OOO=>C6H13OOOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 631 CN
C7H16+R40C6H13OOO=>C6H13OOOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 632 CN
C7H16+R40C6H13OOO=>C6H13OOOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 633 CN
C7H16+R40C6H13OOO=>C6H13OOOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 634 CN
C5H12O+R40C6H13OOO=>C6H13OOOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 635 CN
C5H12O+R40C6H13OOO=>C6H13OOOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 636 CN    -2
C6H14O+R40C6H13OOO=>C6H13OOOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 637 CN
C6H14O+R40C6H13OOO=>C6H13OOOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 638 CN
C6H14O+R40C6H13OOO=>C6H13OOOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 639 CN
C7H16+R41C6H13OOO=>C6H13OOOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 640 CN
C7H16+R41C6H13OOO=>C6H13OOOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 641 CN
C7H16+R41C6H13OOO=>C6H13OOOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 642 CN
C7H16+R41C6H13OOO=>C6H13OOOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 643 CN
C5H12O+R41C6H13OOO=>C6H13OOOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 644 CN
C5H12O+R41C6H13OOO=>C6H13OOOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 645 CN    -2
C6H14O+R41C6H13OOO=>C6H13OOOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 646 CN
C6H14O+R41C6H13OOO=>C6H13OOOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 647 CN
C6H14O+R41C6H13OOO=>C6H13OOOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 648 CN
C7H16+R42C6H13OOO=>C6H13OOOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 649 CN
C7H16+R42C6H13OOO=>C6H13OOOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 650 CN
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C7H16+R42C6H13OOO=>C6H13OOOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 651 CN
C7H16+R42C6H13OOO=>C6H13OOOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 652 CN
C5H12O+R42C6H13OOO=>C6H13OOOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 653 CN
C5H12O+R42C6H13OOO=>C6H13OOOH+R26C5H11O    6.0E+12  0.0  18000.0  ! ME 654 CN    -2
C6H14O+R42C6H13OOO=>C6H13OOOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 655 CN
C6H14O+R42C6H13OOO=>C6H13OOOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 656 CN
C6H14O+R42C6H13OOO=>C6H13OOOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 657 CN

C7H16+R72C4H9OO=>C4H9OOH+R21C7H15    3.0E+12  0.0  17500.0  ! ME 649 CN
C7H16+R72C4H9OO=>C4H9OOH+R22C7H15    6.0E+12  0.0  17500.0  ! ME 650 CN
C7H16+R72C4H9OO=>C4H9OOH+R23C7H15    6.0E+12  0.0  17500.0  ! ME 651 CN
C7H16+R72C4H9OO=>C4H9OOH+R24C7H15    1.2E+13  0.0  20000.0  ! ME 652 CN
C5H12O+R72C4H9OO=>C4H9OOH+R25C5H11O    1.8E+13  0.0  20000.0  ! ME 653 CN
C5H12O+R72C4H9OO=>C4H9OOH+R26C5H11O    6.0E+12  0.0  20000.0  ! ME 654 CN
C6H14O+R72C4H9OO=>C4H9OOH+R27C6H13O    1.8E+13  0.0  20000.0  ! ME 655 CN
C6H14O+R72C4H9OO=>C4H9OOH+R28C6H13O    4.0E+12  0.0  20000.0  ! ME 656 CN
C6H14O+R72C4H9OO=>C4H9OOH+R29C6H13O    6.0E+12  0.0  20000.0  ! ME 657 CN

!   combinations :
R1H+R39C4H9=>C4H10    9.2E+12  0.0  0.0  ! CO 1292 KB
R1H+R325C3H7=>C3H8    9.2E+12  0.0  0.0  ! CO 1293 KB
R2OH+R39C4H9=>C4H9OH    6.2E+12  0.0  0.0  ! CO 1294 KB
R2OH+R325C3H7=>C3H7OH    6.4E+12  0.0  0.0  ! CO 1295 KB
R3O2H+R39C4H9=>C4H9OOH    4.9E+12  0.0  0.0  ! CO 1296 KB
R3O2H+R325C3H7=>C3H7OOH    5.2E+12  0.0  0.0  ! CO 1297 KB
R4CH3+R39C4H9=>C5H12    1.7E+13  0.0  0.0  ! CO 1298 KB
R4CH3+R325C3H7=>C4H10    1.7E+13  0.0  0.0  ! CO 1299 KB
R5CHO+R39C4H9=>C4H9CHO    5.3E+12  0.0  0.0  ! CO 1300 KB
R5CHO+R325C3H7=>C3H7CHO    5.6E+12  0.0  0.0  ! CO 1301 KB
R6CH2OH+R39C4H9=>C5H11OH    5.2E+12  0.0  0.0  ! CO 1302 KB
R6CH2OH+R325C3H7=>C4H9OH    5.5E+12  0.0  0.0  ! CO 1303 KB
R7CH3O+R39C4H9=>C5H12O    5.0E+12  0.0  0.0  ! CO 1304 KB
R7CH3O+R325C3H7=>C4H10O    5.3E+12  0.0  0.0  ! CO 1305 KB
R11C2H5+R39C4H9=>C6H14    5.3E+12  0.0  0.0  ! CO 1306 KB
R11C2H5+R325C3H7=>C5H12    5.6E+12  0.0  0.0  ! CO 1307 KB
R39C4H9+R39C4H9=>C8H18    2.2E+12  0.0  0.0  ! CO 1308 KB
R39C4H9+R325C3H7=>C7H16    4.7E+12  0.0  0.0  ! CO 1309 KB
R325C3H7+R325C3H7=>C6H14    2.5E+12  0.0  0.0  ! CO 1310 KB

!   dismutations :
R30C3H7OO+R3O2H=>C3H7OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1311 CN
R31C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1312 CN
R32C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1313 CN
R33C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1314 CN
R34C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1315 CN
R35C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1316 CN
R37C5H11OOO+R3O2H=>C5H11OOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1317 CN
R38C5H11OOO+R3O2H=>C5H11OOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1318 CN
R40C6H13OOO+R3O2H=>C6H13OOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1319 CN
R41C6H13OOO+R3O2H=>C6H13OOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1320 CN
R42C6H13OOO+R3O2H=>C6H13OOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1321 CN
R67C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1322 CN
R72C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1323 CN
R122C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1324 CN
R198C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1325 CN
R204C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1326 CN
R218C3H7OO+R3O2H=>C3H7OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1327 CN
R249C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1328 CN
R264C4H8OHOO+R3O2H=>C4H8OHOOH+O2    2.0E+11  0.0  -1300.0  ! DI 1329 CN

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!    SECONDARY MECHANISM
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! Hydroperoxide decomposition
C3H5OOHY=>R2OH+HCHO+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 1981
C6H11OOHZ=>R2OH+CH3CHO+C2H4Z+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 1982
C4H7OOHY=>R2OH+CH3CHO+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 1983
C5H9OOHZ=>R2OH+HCHO+C2H4Z+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 1984
C4H9OOH=>R2OH+CH3CHO+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 1985
C3H7OOH=>R2OH+HCHO+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 1986
C7H15OOH=>R2OH+HCHO+2C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 1987
C5H11OOH=>R2OH+HCHO+C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 1988

C6H13OOOH=>R2OH+2HCHO+R11C2H5+C2H4Z   7.0E+14  0.0  42000.0
C5H9OOOHY=>R2OH+HCHO+CH3CHO+R10C2H3V    7.0E+14  0.0  42000.0

C5H11OOOH=>R2OH+2HCHO+R4CH3+C2H4Z   7.0E+14  0.0  42000.0
C4H7OOOHY=>R2OH+2HCHO+R10C2H3V    7.0E+14  0.0  42000.0


! Dihydroperoxide decomposition
C4H6O4H2Y=>R2OH+R2OH+HCHO+C2H2+HCHO    7.0E+14  0.0  42000.0  ! DKD 1989
C4H6O4H2Y=>R2OH+R2OH+CH2COZ+CH3CHO    7.0E+14  0.0  42000.0  ! DKD 1990
C4H6O4H2Y=>R2OH+R3O2H+CH2COZ+C2H4Z    7.0E+14  0.0  42000.0  ! DKD 1991

! Ketohydroperoxide decomposition
C2H5COOOH=>R2OH+HCHO+B2CO+R4CH3    7.0E+14  0.0  42000.0  ! DK1 1992
C6H13COOOH=>R2OH+HCHO+B2CO+2C2H4Z+R4CH3    7.0E+14  0.0  42000.0  ! DK1 1993
C3H7COOOH=>R2OH+HCHO+B2CO+R11C2H5    7.0E+14  0.0  42000.0  ! DK1 1994
C4H9COOOH=>R2OH+HCHO+B2CO+C2H4Z+R4CH3    7.0E+14  0.0  42000.0  ! DK1 1995
C5H11OCOOOH=>R2OH+2CH3CHO+B2CO+R4CH3    7.0E+14  0.0  42000.0  ! DK1 ether

! Aldohydroperoxide decomposition
C2H4CHOOOH=>R2OH+CH3CHO+R5CHO    7.0E+14  0.0  42000.0  ! DK2 1996
C3H6CHOOOH=>R2OH+CH3CHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DK2 1997
C6H12CHOOOH=>R2OH+CH3CHO+2C2H4Z+R5CHO    7.0E+14  0.0  42000.0  ! DK2 1998
C4H8CHOOOH=>R2OH+CH3CHO+C2H4Z+R5CHO    7.0E+14  0.0  42000.0  ! DK2 1999
C4H8OCHOOOH=>R2OH+2CH3CHO+R5CHO    7.0E+14  0.0  42000.0  ! DK2 ether
C5H10OCHOOOH=>R2OH+2CH3CHO+R13CH2CHO   7.0E+14  0.0  42000.0  ! DK2 ether

! Hydroperoxy ring decomposition
C3H5O#3OOH=>R2OH+HCHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DHC 2000
C3H5O#4OOH=>R2OH+HCHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DHC 2001
C4H7O#3OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2002
C4H7O#4OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2003
C4H7O#5OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2004
C7H13O#3OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2005
C7H13O#4OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2006
C7H13O#5OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2007
C7H13O#6OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2008
C5H9O#3OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2009
C5H9O#4OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2010
C5H9O#5OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2011
C5H9O#6OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2012

! Alcane reactions
C3H8+R1H=>H2+R4CH3+C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2013
C3H8+R2OH=>H2O+R4CH3+C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2014
C3H8+R3O2H=>H2O2+R4CH3+C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2015
C3H8+R4CH3=>CH4+R4CH3+C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2016
C3H8+R11C2H5=>C2H6+R4CH3+C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2017
C4H10+R1H=>H2+R11C2H5+C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2018
C4H10+R2OH=>H2O+R11C2H5+C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2019
C4H10+R3O2H=>H2O2+R11C2H5+C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2020
C4H10+R4CH3=>CH4+R11C2H5+C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2021
C4H10+R11C2H5=>C2H6+R11C2H5+C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2022
C5H12+R1H=>H2+R4CH3+2C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2023
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C5H12+R2OH=>H2O+R4CH3+2C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2024
C5H12+R3O2H=>H2O2+R4CH3+2C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2025
C5H12+R4CH3=>CH4+R4CH3+2C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2026
C5H12+R11C2H5=>C2H6+R4CH3+2C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2027
C6H14+R1H=>H2+R11C2H5+2C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2028
C6H14+R2OH=>H2O+R11C2H5+2C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2029
C6H14+R3O2H=>H2O2+R11C2H5+2C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2030
C6H14+R4CH3=>CH4+R11C2H5+2C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2031
C6H14+R11C2H5=>C2H6+R11C2H5+2C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2032
C8H18+R1H=>H2+R11C2H5+3C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2033
C8H18+R2OH=>H2O+R11C2H5+3C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2034
C8H18+R3O2H=>H2O2+R11C2H5+3C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2035
C8H18+R4CH3=>CH4+R11C2H5+3C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2036
C8H18+R11C2H5=>C2H6+R11C2H5+3C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2037

! O-ring decomposition

C3H6O#3+R1H=>H2+CH2COZ+R4CH3    2.7E+07  2.0  5000.0  ! ??? 2038
C3H6O#3+R2OH=>H2O+CH2COZ+R4CH3    7.8E+06  2.0  -765.0  ! ??? 2039
C3H6O#3+R3O2H=>H2O2+CH2COZ+R4CH3    1.2E+12  0.0  15500.0  ! ??? 2040
C3H6O#3+R4CH3=>CH4+CH2COZ+R4CH3    6.0E+11  0.0  9600.0  ! ??? 2041
C3H6O#3+R11C2H5=>C2H6+CH2COZ+R4CH3    6.0E+11  0.0  11000.0  ! ??? 2042
C4H8O#3+R1H=>H2+CH2COZ+R11C2H5    2.7E+07  2.0  5000.0  ! ??? 2043
C4H8O#3+R2OH=>H2O+CH2COZ+R11C2H5    7.8E+06  2.0  -765.0  ! ??? 2044
C4H8O#3+R3O2H=>H2O2+CH2COZ+R11C2H5    1.2E+12  0.0  15500.0  ! ??? 2045
C4H8O#3+R4CH3=>CH4+CH2COZ+R11C2H5    6.0E+11  0.0  9600.0  ! ??? 2046
C4H8O#3+R11C2H5=>C2H6+CH2COZ+R11C2H5    6.0E+11  0.0  11000.0  ! ??? 2047
C7H14O#3+R1H=>H2+CH2COZ+R4CH3+2C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2048
C7H14O#3+R2OH=>H2O+CH2COZ+R4CH3+2C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2049
C7H14O#3+R3O2H=>H2O2+CH2COZ+R4CH3+2C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2050
C7H14O#3+R4CH3=>CH4+CH2COZ+R4CH3+2C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2051
C7H14O#3+R11C2H5=>C2H6+CH2COZ+R4CH3+2C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2052
C5H10O#3+R1H=>H2+CH2COZ+R4CH3+C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2053
C5H10O#3+R2OH=>H2O+CH2COZ+R4CH3+C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2054
C5H10O#3+R3O2H=>H2O2+CH2COZ+R4CH3+C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2055
C5H10O#3+R4CH3=>CH4+CH2COZ+R4CH3+C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2056
C5H10O#3+R11C2H5=>C2H6+CH2COZ+R4CH3+C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2057
C6H12O#3+R1H=>H2+CH2COZ+R11C2H5+C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2058
C6H12O#3+R2OH=>H2O+CH2COZ+R11C2H5+C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2059
C6H12O#3+R3O2H=>H2O2+CH2COZ+R11C2H5+C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2060
C6H12O#3+R4CH3=>CH4+CH2COZ+R11C2H5+C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2061
C6H12O#3+R11C2H5=>C2H6+CH2COZ+R11C2H5+C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2062

! Metatheses of oxiranes and furanes
C3H6O#4+R1H=>H2+.C3H5O#4    2.7E+07  2.0  5000.0  ! ??? 2063
C3H6O#4+R2OH=>H2O+.C3H5O#4    7.8E+06  2.0  -765.0  ! ??? 2064
C3H6O#4+R3O2H=>H2O2+.C3H5O#4    1.2E+12  0.0  15500.0  ! ??? 2065
C3H6O#4+R4CH3=>CH4+.C3H5O#4    6.0E+11  0.0  9600.0  ! ??? 2066
C3H6O#4+R11C2H5=>C2H6+.C3H5O#4    6.0E+11  0.0  11000.0  ! ??? 2067
C4H8O#4+R1H=>H2+.C4H7O#4    2.7E+07  2.0  5000.0  ! ??? 2068
C4H8O#4+R2OH=>H2O+.C4H7O#4    7.8E+06  2.0  -765.0  ! ??? 2069
C4H8O#4+R3O2H=>H2O2+.C4H7O#4    1.2E+12  0.0  15500.0  ! ??? 2070
C4H8O#4+R4CH3=>CH4+.C4H7O#4    6.0E+11  0.0  9600.0  ! ??? 2071
C4H8O#4+R11C2H5=>C2H6+.C4H7O#4    6.0E+11  0.0  11000.0  ! ??? 2072
C4H8O#5+R1H=>H2+.C4H7O#5    2.7E+07  2.0  5000.0  ! ??? 2073
C4H8O#5+R2OH=>H2O+.C4H7O#5    7.8E+06  2.0  -765.0  ! ??? 2074
C4H8O#5+R3O2H=>H2O2+.C4H7O#5    1.2E+12  0.0  15500.0  ! ??? 2075
C4H8O#5+R4CH3=>CH4+.C4H7O#5    6.0E+11  0.0  9600.0  ! ??? 2076
C4H8O#5+R11C2H5=>C2H6+.C4H7O#5    6.0E+11  0.0  11000.0  ! ??? 2077
C7H14O#4+R1H=>H2+.C7H13O#4    2.7E+07  2.0  5000.0  ! ??? 2078
C7H14O#4+R2OH=>H2O+.C7H13O#4    7.8E+06  2.0  -765.0  ! ??? 2079
C7H14O#4+R3O2H=>H2O2+.C7H13O#4    1.2E+12  0.0  15500.0  ! ??? 2080
C7H14O#4+R4CH3=>CH4+.C7H13O#4    6.0E+11  0.0  9600.0  ! ??? 2081
C7H14O#4+R11C2H5=>C2H6+.C7H13O#4    6.0E+11  0.0  11000.0  ! ??? 2082
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C7H14O#5+R1H=>H2+.C7H13O#5    2.7E+07  2.0  5000.0  ! ??? 2083
C7H14O#5+R2OH=>H2O+.C7H13O#5    7.8E+06  2.0  -765.0  ! ??? 2084
C7H14O#5+R3O2H=>H2O2+.C7H13O#5    1.2E+12  0.0  15500.0  ! ??? 2085
C7H14O#5+R4CH3=>CH4+.C7H13O#5    6.0E+11  0.0  9600.0  ! ??? 2086
C7H14O#5+R11C2H5=>C2H6+.C7H13O#5    6.0E+11  0.0  11000.0  ! ??? 2087
C7H14O#6+R1H=>H2+.C7H13O#6    2.7E+07  2.0  5000.0  ! ??? 2088
C7H14O#6+R2OH=>H2O+.C7H13O#6    7.8E+06  2.0  -765.0  ! ??? 2089
C7H14O#6+R3O2H=>H2O2+.C7H13O#6    1.2E+12  0.0  15500.0  ! ??? 2090
C7H14O#6+R4CH3=>CH4+.C7H13O#6    6.0E+11  0.0  9600.0  ! ??? 2091
C7H14O#6+R11C2H5=>C2H6+.C7H13O#6    6.0E+11  0.0  11000.0  ! ??? 2092
C5H10O#4+R1H=>H2+.C5H9O#4    2.7E+07  2.0  5000.0  ! ??? 2093
C5H10O#4+R2OH=>H2O+.C5H9O#4    7.8E+06  2.0  -765.0  ! ??? 2094
C5H10O#4+R3O2H=>H2O2+.C5H9O#4    1.2E+12  0.0  15500.0  ! ??? 2095
C5H10O#4+R4CH3=>CH4+.C5H9O#4    6.0E+11  0.0  9600.0  ! ??? 2096
C5H10O#4+R11C2H5=>C2H6+.C5H9O#4    6.0E+11  0.0  11000.0  ! ??? 2097
C5H10O#5+R1H=>H2+.C5H9O#5    2.7E+07  2.0  5000.0  ! ??? 2098
C5H10O#5+R2OH=>H2O+.C5H9O#5    7.8E+06  2.0  -765.0  ! ??? 2099
C5H10O#5+R3O2H=>H2O2+.C5H9O#5    1.2E+12  0.0  15500.0  ! ??? 2100
C5H10O#5+R4CH3=>CH4+.C5H9O#5    6.0E+11  0.0  9600.0  ! ??? 2101
C5H10O#5+R11C2H5=>C2H6+.C5H9O#5    6.0E+11  0.0  11000.0  ! ??? 2102
C5H10O#6+R1H=>H2+.C5H9O#6    2.7E+07  2.0  5000.0  ! ??? 2103
C5H10O#6+R2OH=>H2O+.C5H9O#6    7.8E+06  2.0  -765.0  ! ??? 2104
C5H10O#6+R3O2H=>H2O2+.C5H9O#6    1.2E+12  0.0  15500.0  ! ??? 2105
C5H10O#6+R4CH3=>CH4+.C5H9O#6    6.0E+11  0.0  9600.0  ! ??? 2106
C5H10O#6+R11C2H5=>C2H6+.C5H9O#6    6.0E+11  0.0  11000.0  ! ??? 2107

! decompositions of cyclo-ether radicals
.C3H5O#4=>R5CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2108
.C4H7O#4=>R13CH2CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2109
.C4H7O#5=>R13CH2CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2110
.C7H13O#4=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2111
.C7H13O#5=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2112
.C7H13O#6=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2113
.C5H9O#4=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2114
.C5H9O#5=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2115
.C5H9O#6=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2116

! Addition of oxygen on cyclo-ether radicals
.C3H5O#4+O2=>.OOC3H5O#4    2.2E+19  -2.5  0.0  ! ??? 2117
.C4H7O#4+O2=>.OOC4H7O#4    2.2E+19  -2.5  0.0  ! ??? 2118
.C4H7O#5+O2=>.OOC4H7O#5    2.2E+19  -2.5  0.0  ! ??? 2119
.C7H13O#4+O2=>.OOC7H13O#4    2.2E+19  -2.5  0.0  ! ??? 2120
.C7H13O#5+O2=>.OOC7H13O#5    2.2E+19  -2.5  0.0  ! ??? 2121
.C7H13O#6+O2=>.OOC7H13O#6    2.2E+19  -2.5  0.0  ! ??? 2122
.C5H9O#4+O2=>.OOC5H9O#4    2.2E+19  -2.5  0.0  ! ??? 2123
.C5H9O#5+O2=>.OOC5H9O#5    2.2E+19  -2.5  0.0  ! ??? 2124
.C5H9O#6+O2=>.OOC5H9O#6    2.2E+19  -2.5  0.0  ! ??? 2125
.OOC3H5O#4=>.C3H5O#4+ O2    5.0E+22  -2.5  36000.0  ! ??? 2126
.OOC4H7O#4=>.C4H7O#4+ O2    5.0E+22  -2.5  36000.0  ! ??? 2127
.OOC4H7O#5=>.C4H7O#5+ O2    5.0E+22  -2.5  36000.0  ! ??? 2128
.OOC7H13O#4=>.C7H13O#4+ O2    5.0E+22  -2.5  36000.0  ! ??? 2129
.OOC7H13O#5=>.C7H13O#5+ O2    5.0E+22  -2.5  36000.0  ! ??? 2130
.OOC7H13O#6=>.C7H13O#6+ O2    5.0E+22  -2.5  36000.0  ! ??? 2131
.OOC5H9O#4=>.C5H9O#4+ O2    5.0E+22  -2.5  36000.0  ! ??? 2132
.OOC5H9O#5=>.C5H9O#5+ O2    5.0E+22  -2.5  36000.0  ! ??? 2133
.OOC5H9O#6=>.C5H9O#6+ O2    5.0E+22  -2.5  36000.0  ! ??? 2134

! Isomerization of peroxy-radicals
.OOC3H5O#4=>.C3H4O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2135
.OOC4H7O#4=>.C4H6O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2136
.OOC4H7O#5=>.C4H6O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2137
.OOC7H13O#4=>.C7H12O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2138
.OOC7H13O#5=>.C7H12O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2139
.OOC7H13O#6=>.C7H12O#6OOH    8.0E+13  0.0  25500.0  ! ??? 2140
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.OOC5H9O#4=>.C5H8O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2141
.OOC5H9O#5=>.C5H8O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2142
.OOC5H9O#6=>.C5H8O#6OOH    8.0E+13  0.0  25500.0  ! ??? 2143
.C3H4O#4OOH=>.OOC3H5O#4    4.8E+12  0.0  19000.0  ! ??? 2144
.C4H6O#4OOH=>.OOC4H7O#4    4.8E+12  0.0  19000.0  ! ??? 2145
.C4H6O#5OOH=>.OOC4H7O#5    4.8E+12  0.0  19000.0  ! ??? 2146
.C7H12O#4OOH=>.OOC7H13O#4    4.8E+12  0.0  19000.0  ! ??? 2147
.C7H12O#5OOH=>.OOC7H13O#5    4.8E+12  0.0  19000.0  ! ??? 2148
.C7H12O#6OOH=>.OOC7H13O#6    4.8E+12  0.0  19000.0  ! ??? 2149
.C5H8O#4OOH=>.OOC5H9O#4    4.8E+12  0.0  19000.0  ! ??? 2150
.C5H8O#5OOH=>.OOC5H9O#5    4.8E+12  0.0  19000.0  ! ??? 2151
.C5H8O#6OOH=>.OOC5H9O#6    4.8E+12  0.0  19000.0  ! ??? 2152

!Addition of oxygen on cyclo-peroxy radicals
.C3H4O#4OOH+O2=>.OOC3H4O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2153
.C4H6O#4OOH+O2=>.OOC4H6O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2154
.C4H6O#5OOH+O2=>.OOC4H6O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2155
.C7H12O#4OOH+O2=>.OOC7H12O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2156
.C7H12O#5OOH+O2=>.OOC7H12O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2157
.C7H12O#6OOH+O2=>.OOC7H12O#6OOH    2.2E+19  -2.5  0.0  ! ??? 2158
.C5H8O#4OOH+O2=>.OOC5H8O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2159
.C5H8O#5OOH+O2=>.OOC5H8O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2160
.C5H8O#6OOH+O2=>.OOC5H8O#6OOH    2.2E+19  -2.5  0.0  ! ??? 2161
.OOC3H4O#4OOH=>.C3H4O#4OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2162
.OOC4H6O#4OOH=>.C4H6O#4OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2163
.OOC4H6O#5OOH=>.C4H6O#5OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2164
.OOC7H12O#4OOH=>.C7H12O#4OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2165
.OOC7H12O#5OOH=>.C7H12O#5OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2166
.OOC7H12O#6OOH=>.C7H12O#6OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2167
.OOC5H8O#4OOH=>.C5H8O#4OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2168
.OOC5H8O#5OOH=>.C5H8O#5OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2169
.OOC5H8O#6OOH=>.C5H8O#6OOH+ O2    5.0E+22  -2.5  36000.0  ! ??? 2170

! Formation of cyclo-ether ketohydroperoxydes
.OOC3H4O#4OOH=>R2OH+C2H3O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2171
.OOC4H6O#4OOH=>R2OH+C3H5O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2172
.OOC4H6O#5OOH=>R2OH+C3H5O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2173
.OOC7H12O#4OOH=>R2OH+C6H11O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2174
.OOC7H12O#5OOH=>R2OH+C6H11O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2175
.OOC7H12O#6OOH=>R2OH+C6H11O#6COOOH    1.0E+09  0.0  7500.0  ! ??? 2176
.OOC5H8O#4OOH=>R2OH+C4H7O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2177
.OOC5H8O#5OOH=>R2OH+C4H7O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2178
.OOC5H8O#6OOH=>R2OH+C4H7O#6COOOH    1.0E+09  0.0  7500.0  ! ??? 2179

! Decomposition of cyclo-ether ketohydroperoxydes
C2H3O#4COOOH=>R2OH+CO2+R13CH2CHO    7.0E+14  0.0  42000.0  ! ??? 2180
C3H5O#4COOOH=>R2OH+CO2+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2181
C3H5O#5COOOH=>R2OH+CO2+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2182
C6H11O#4COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2183
C6H11O#5COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2184
C6H11O#6COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2185
C4H7O#4COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2186
C4H7O#5COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2187
C4H7O#6COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2188

! Olefin reactions to product products of the base
C3H6Y+R1H=>C2H4Z+R4CH3    7.2E+12  0.0  2900.0  ! ROL 1786
C3H6Y+R4CH3=>C2H4Z+R11C2H5    9.6E+10  0.0  8000.0  ! ROL 1787
C4H8Y+R1H=>C2H4Z+R11C2H5             7.2E+12  0.0  2900.0  ! ROL 208
C4H8Y+R1H=>C3H6Y+R4CH3               7.2E+12  0.0  1300.0  ! ROL 208'
C4H8Y+R4CH3=>C3H6Y+R11C2H5           9.6E+10  0.0  8000.0  ! ROL 209
C7H14Z+R1H=>3C2H4Z+R4CH3             7.2E+12  0.0  2900.0  ! ROL 210
C7H14Z+R1H=>C3H6Y+R11C2H5+C2H4Z      7.2E+12  0.0  1300.0  ! ROL 210'
C7H14Z+R4CH3=>C3H6Y+R4CH3+2C2H4Z     9.6E+10  0.0  8000.0  ! ROL 211
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C6H12Z+R1H=>2C2H4Z+R11C2H5           7.2E+12  0.0  2900.0  ! ROL 212
C6H12Z+R1H=>C3H6Y+R4CH3+C2H4Z        7.2E+12  0.0  1300.0  ! ROL 212'
C6H12Z+R4CH3=>C3H6Y+R11C2H5+C2H4Z    9.6E+10  0.0  8000.0  ! ROL 213
C5H10Z+R1H=>2C2H4Z+R4CH3             7.2E+12  0.0  2900.0  ! ROL 218
C5H10Z+R1H=>C3H6Y+R11C2H5            7.2E+12  0.0  1300.0  ! ROL 218'
C5H10Z+R4CH3=>C3H6Y+R4CH3+C2H4Z      9.6E+10  0.0  8000.0  ! ROL 219

!  olefin to aldehydes
C3H6Y+R2OH=>R4CH3+CH3CHO    1.4E+12  0.0  -900.0  ! ALD 179
C4H8Y+R2OH=>R4CH3+C2H5CHO    1.4E+12  0.0  -900.0  ! ALD 180
C7H14Z+R2OH=>R4CH3+C5H11CHO    1.4E+12  0.0  -900.0  ! ALD 181
C6H12Z+R2OH=>R4CH3+C4H9CHO    1.4E+12  0.0  -900.0  ! ALD 183
C5H10Z+R2OH=>R4CH3+C3H7CHO    1.4E+12  0.0  -900.0  ! ALD 184

!  olefin to alkohols
C4H8Y+R2OH=>HCHO+C2H4Z+R4CH3    1.4E+12  0.0  -900.0  ! FOH 185
C7H14Z+R2OH=>HCHO+2C2H4Z+R11C2H5    1.4E+12  0.0  -900.0  ! FOH 186
C6H12Z+R2OH=>HCHO+2C2H4Z+R4CH3    1.4E+12  0.0  -900.0  ! FOH 188
C5H10Z+R2OH=>HCHO+C2H4Z+R11C2H5    1.4E+12  0.0  -900.0  ! FOH 189

!   olefin to dienes
!   reactions ajoutees pour augmenter la formation du butadiene
!   les olefines ne donnent plus un diene par perte de CH3 mais que du butadiene
!   valeurs cinetiques modifiees par rapport a exgas
C7H14Z+R1H=>H2+C4H6Z2+C2H4Z+R4CH3    8.9E+06  2.0  3000.0  ! FYZ 237
C7H14Z+R2OH=>H2O+C4H6Z2+C2H4Z+R4CH3    2.57E+06  2.0  -2700.0  ! FZZ 238
C7H14Z+R3O2H=>H2O2+C4H6Z2+C2H4Z+R4CH3    4.0E+11  0.0  13500.0  ! FZZ 239
C7H14Z+R4CH3=>CH4+C4H6Z2+C2H4Z+R4CH3    2.0E+11  0.0  7500.0  ! FZZ 240
C7H14Z+R11C2H5=>C2H6+C4H6Z2+C2H4Z+R4CH3    2.0E+11  0.0  9000.0  ! FZZ 241
C7H14Z+B1O=>R2OH+C4H6Z2+R4CH3+C2H4Z   4.0E+13  0.0  3200.0
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    8.9E+06  2.0  3000.0  ! FZZ 242
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    2.57E+06  2.0  -2700.0  ! FZZ 243
C6H12Z+R3O2H=>H2O2+C4H6Z2+R11C2H5    4.0E+11  0.0  13500.0  ! FZZ 244
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    2.0E+11  0.0  7500.0  ! FZZ 245
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    2.0E+11  0.0  9000.0  ! FZZ 246
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5   4.0E+13  0.0  3200.0
C5H10Z+R1H=>H2+R4CH3+C4H6Z2    8.9E+06  2.0  3000.0  ! FZZ 257
C5H10Z+R2OH=>H2O+R4CH3+C4H6Z2    2.57E+06  2.0  -2700.0  ! FZZ 258
C5H10Z+R3O2H=>H2O2+R4CH3+C4H6Z2    4.0E+11  0.0  13500.0  ! FZZ 259
C5H10Z+R4CH3=>CH4+R4CH3+C4H6Z2    2.0E+11  0.0  7500.0  ! FZZ 260
C5H10Z+R11C2H5=>C2H6+R4CH3+C4H6Z2    2.0E+11  0.0  9000.0  ! FZZ 261
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3   4.0E+13  0.0  3200.0

!  epoxy formation
C3H6Y+R3O2H=>R2OH+C3H6O#3    1.0E+12  0.0  14400.0  ! FCY 2223
C4H8Y+R3O2H=>R2OH+C4H8O#3    1.0E+12  0.0  14400.0  ! FCY 2224
C5H10Z+R3O2H=>R2OH+C5H10O#3    1.0E+12  0.0  14400.0  ! FCY 2225
C6H12Z+R3O2H=>R2OH+C6H12O#3    1.0E+12  0.0  14400.0  ! FCY 2226
C7H14Z+R3O2H=>R2OH+C7H14O#3    1.0E+12  0.0  14400.0  ! FCY 2227

! Alkohol reactions
C3H7OH+R1H=>H2+R2OH+C3H6Y    9.0E+06  2.0  5000.0  ! AL 1825
C3H7OH+R1H=>H2+R4CH3+CH3CHO    4.2E+06  2.0  2400.0  ! AL 1826
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    1.3E+09  1.3  700.0  ! AL 1827
C3H7OH+R2OH=>H2O+R4CH3+CH3CHO    4.0E+12  0.0  443.0  ! AL 1828
C3H7OH+R3O2H=>H2O2+R2OH+C3H6Y    4.0E+11  0.0  15500.0  ! AL 1829
C3H7OH+R3O2H=>H2O2+R4CH3+CH3CHO    1.0E+12  0.0  14000.0  ! AL 1830
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    2.0E+11  0.0  9600.0  ! AL 1831
C3H7OH+R4CH3=>CH4+R4CH3+CH3CHO    1.0E+11  0.0  7600.0  ! AL 1832
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    2.0E+11  0.0  11000.0  ! AL 1833
C3H7OH+R11C2H5=>C2H6+R4CH3+CH3CHO    1.0E+11  0.0  9200.0  ! AL 1834
C4H9OH+R1H=>H2+R2OH+C4H8Y    9.0E+06  2.0  5000.0  ! AL 1835
C4H9OH+R1H=>H2+R4CH3+C2H5CHO    4.2E+06  2.0  2400.0  ! AL 1836
C4H9OH+R1H=>H2+R4CH3+C2H6CO    4.2E+06  2.0  2400.0  ! AL 1837
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C4H9OH+R2OH=>H2O+R2OH+C4H8Y    1.3E+09  1.3  700.0  ! AL 1838
C4H9OH+R2OH=>H2O+R4CH3+C2H5CHO    4.0E+12  0.0  443.0  ! AL 1839
C4H9OH+R2OH=>H2O+R4CH3+C2H6CO    4.0E+12  0.0  443.0  ! AL 1840
C4H9OH+R3O2H=>H2O2+R2OH+C4H8Y    4.0E+11  0.0  15500.0  ! AL 1841
C4H9OH+R3O2H=>H2O2+R4CH3+C2H5CHO    1.0E+12  0.0  14000.0  ! AL 1842
C4H9OH+R3O2H=>H2O2+R4CH3+C2H6CO    1.0E+12  0.0  14000.0  ! AL 1843
C4H9OH+R4CH3=>CH4+R2OH+C4H8Y    2.0E+11  0.0  9600.0  ! AL 1844
C4H9OH+R4CH3=>CH4+R4CH3+C2H5CHO    1.0E+11  0.0  7600.0  ! AL 1845
C4H9OH+R4CH3=>CH4+R4CH3+C2H6CO    1.0E+11  0.0  7600.0  ! AL 1846
C4H9OH+R11C2H5=>C2H6+R2OH+C4H8Y    2.0E+11  0.0  11000.0  ! AL 1847
C4H9OH+R11C2H5=>C2H6+R4CH3+C2H5CHO    1.0E+11  0.0  9200.0  ! AL 1848
C4H9OH+R11C2H5=>C2H6+R4CH3+C2H6CO    1.0E+11  0.0  9200.0  ! AL 1849
C5H11OH+R1H=>H2+R2OH+C5H10Z    9.0E+06  2.0  5000.0  ! AL 768
C5H11OH+R1H=>H2+R4CH3+C3H7CHO    4.2E+06  2.0  2400.0  ! AL 769
C5H11OH+R1H=>H2+R4CH3+C3H8CO    4.2E+06  2.0  2400.0  ! AL 770
C5H11OH+R2OH=>H2O+R2OH+C5H10Z    1.3E+09  1.3  700.0  ! AL 771
C5H11OH+R2OH=>H2O+R4CH3+C3H7CHO    4.0E+12  0.0  443.0  ! AL 772
C5H11OH+R2OH=>H2O+R4CH3+C3H8CO    4.0E+12  0.0  443.0  ! AL 773
C5H11OH+R3O2H=>H2O2+R2OH+C5H10Z    4.0E+11  0.0  15500.0  ! AL 774
C5H11OH+R3O2H=>H2O2+R4CH3+C3H7CHO    1.0E+12  0.0  14000.0  ! AL 775
C5H11OH+R3O2H=>H2O2+R4CH3+C3H8CO    1.0E+12  0.0  14000.0  ! AL 776
C5H11OH+R4CH3=>CH4+R2OH+C5H10Z    2.0E+11  0.0  9600.0  ! AL 777
C5H11OH+R4CH3=>CH4+R4CH3+C3H7CHO    1.0E+11  0.0  7600.0  ! AL 778
C5H11OH+R4CH3=>CH4+R4CH3+C3H8CO    1.0E+11  0.0  7600.0  ! AL 779
C5H11OH+R11C2H5=>C2H6+R2OH+C5H10Z    2.0E+11  0.0  11000.0  ! AL 780
C5H11OH+R11C2H5=>C2H6+R4CH3+C3H7CHO    1.0E+11  0.0  9200.0  ! AL 781
C5H11OH+R11C2H5=>C2H6+R4CH3+C3H8CO    1.0E+11  0.0  9200.0  ! AL 782
C4H8OHOOH+R1H=>H2+R2OH+C4H7OOHY    9.0E+06  2.0  5000.0  ! AL 783
C4H8OHOOH+R1H=>H2+R4CH3+C2H4CHOOOH    4.2E+06  2.0  2400.0  ! AL 784
C4H8OHOOH+R1H=>H2+R4CH3+C2H5COOOH    4.2E+06  2.0  2400.0  ! AL 785
C4H8OHOOH+R2OH=>H2O+R2OH+C4H7OOHY    1.3E+09  1.3  700.0  ! AL 786
C4H8OHOOH+R2OH=>H2O+R4CH3+C2H4CHOOOH    4.0E+12  0.0  443.0  ! AL 787
C4H8OHOOH+R2OH=>H2O+R4CH3+C2H5COOOH    4.0E+12  0.0  443.0  ! AL 788
C4H8OHOOH+R3O2H=>H2O2+R2OH+C4H7OOHY    4.0E+11  0.0  15500.0  ! AL 789
C4H8OHOOH+R3O2H=>H2O2+R4CH3+C2H4CHOOOH    1.0E+12  0.0  14000.0  ! AL 790
C4H8OHOOH+R3O2H=>H2O2+R4CH3+C2H5COOOH    1.0E+12  0.0  14000.0  ! AL 791
C4H8OHOOH+R4CH3=>CH4+R2OH+C4H7OOHY    2.0E+11  0.0  9600.0  ! AL 792
C4H8OHOOH+R4CH3=>CH4+R4CH3+C2H4CHOOOH    1.0E+11  0.0  7600.0  ! AL 793
C4H8OHOOH+R4CH3=>CH4+R4CH3+C2H5COOOH    1.0E+11  0.0  7600.0  ! AL 794
C4H8OHOOH+R11C2H5=>C2H6+R2OH+C4H7OOHY    2.0E+11  0.0  11000.0  ! AL 795
C4H8OHOOH+R11C2H5=>C2H6+R4CH3+C2H4CHOOOH    1.0E+11  0.0  9200.0  ! AL 796
C4H8OHOOH+R11C2H5=>C2H6+R4CH3+C2H5COOOH    1.0E+11  0.0  9200.0  ! AL 797

! Metathesis with YH
C3H6Y+R1H=>.C3H5Y+H2    1.7E+05  2.5  2490.0  ! MES 2228
C3H6Y+R2OH=>.C3H5Y+H2O    3.1E+06  2.0  -300.0  ! MES 2229
C3H6Y+R3O2H=>.C3H5Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2230
C3H6Y+R4CH3=>.C3H5Y+CH4    2.2E+00  3.5  5675.0  ! MES 2231
C3H6Y+R11C2H5=>.C3H5Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2232
C4H8Y+R1H=>.C4H7Y+H2    1.7E+05  2.5  2490.0  ! MES 2233
C4H8Y+R2OH=>.C4H7Y+H2O    3.1E+06  2.0  -300.0  ! MES 2234
C4H8Y+R3O2H=>.C4H7Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2235
C4H8Y+R4CH3=>.C4H7Y+CH4    2.2E+00  3.5  5675.0  ! MES 2236
C4H8Y+R11C2H5=>.C4H7Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2237
C3H6Y+B1O=>.C3H5Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2243
C4H8Y+B1O=>.C4H7Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2244

! Addition of .Y on YH
.C3H5Y+C5H10Z=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2246
.C3H5Y+C4H8Y=>R4CH3+C2H2+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2247
.C3H5Y+C3H6Y=>R10C2H3V+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2248
.C4H7Y+C5H10Z=>R4CH3+C2H2+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2249
.C4H7Y+C4H8Y=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2250
.C4H7Y+C3H6Y=>R4CH3+C2H2+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2251
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.C5H9Y+C5H10Z=>R10C2H3V+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2252
.C5H9Y+C4H8Y=>R4CH3+C2H2+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2253
.C5H9Y+C3H6Y=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2254

! Aldehydes metathesis
C2H5CHO+R1H=>H2+.COC2H5    4.0E+13  0.0  4200.0  ! ALD 2255
C2H5CHO+R2OH=>H2O+.COC2H5    4.2E+12  0.0  500.0  ! ALD 2256
C2H5CHO+R4CH3=>CH4+.COC2H5    2.0E-06  5.6  2500.0  ! ALD 2257
C2H5CHO+R11C2H5=>C2H6+.COC2H5    1.3E+12  0.0  8500.0  ! ALD 2258
C3H7CHO+R1H=>H2+.COC3H7    4.0E+13  0.0  4200.0  ! ALD 2259
C3H7CHO+R2OH=>H2O+.COC3H7    4.2E+12  0.0  500.0  ! ALD 2260
C3H7CHO+R4CH3=>CH4+.COC3H7    2.0E-06  5.6  2500.0  ! ALD 2261
C3H7CHO+R11C2H5=>C2H6+.COC3H7    1.3E+12  0.0  8500.0  ! ALD 2262
C4H9CHO+R1H=>H2+.COC4H9    4.0E+13  0.0  4200.0  ! ALD 2263
C4H9CHO+R2OH=>H2O+.COC4H9    4.2E+12  0.0  500.0  ! ALD 2264
C4H9CHO+R4CH3=>CH4+.COC4H9    2.0E-06  5.6  2500.0  ! ALD 2265
C4H9CHO+R11C2H5=>C2H6+.COC4H9    1.3E+12  0.0  8500.0  ! ALD 2266
C6H13CHO+R1H=>H2+.COC6H13    4.0E+13  0.0  4200.0  ! ALD 2267
C6H13CHO+R2OH=>H2O+.COC6H13    4.2E+12  0.0  500.0  ! ALD 2268
C6H13CHO+R4CH3=>CH4+.COC6H13    2.0E-06  5.6  2500.0  ! ALD 2269
C6H13CHO+R11C2H5=>C2H6+.COC6H13    1.3E+12  0.0  8500.0  ! ALD 2270
C5H11CHO+R1H=>H2+.COC5H11    4.0E+13  0.0  4200.0  ! ALD 2271
C5H11CHO+R2OH=>H2O+.COC5H11    4.2E+12  0.0  500.0  ! ALD 2272
C5H11CHO+R4CH3=>CH4+.COC5H11    2.0E-06  5.6  2500.0  ! ALD 2273
C5H11CHO+R11C2H5=>C2H6+.COC5H11    1.3E+12  0.0  8500.0  ! ALD 2274

! Ketones reactions
C3H8CO+R1H=>CH3CHO+R11C2H5    7.0E+00  4.0  1300.0  ! FCO 2275
C3H8CO+R4CH3=>CH3CHO+R4CH3+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2276
C6H14CO+R1H=>C3H8CO+R4CH3+C2H4Z    7.0E+00  4.0  1300.0  ! FCO 2277
C6H14CO+R4CH3=>C3H8CO+R11C2H5+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2278
C4H10CO+R1H=>C2H6CO+R11C2H5    7.0E+00  4.0  1300.0  ! FCO 2279
C4H10CO+R4CH3=>C2H6CO+R4CH3+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2280


! Acid formation
C6H14CO+R2OH=>C3H7COOH+R4CH3+C2H4Z    6.0E+11  0.0  0.0  ! FAC 2281
C4H10CO+R2OH=>C2H5COOH+R11C2H5    6.0E+11  0.0  0.0  ! FAC 2282

! Acid metathesis
C3H7COOH+R1H=>.COOC3H7+H2    4.2E+06  2.1  4900.0  ! MAC 2283
C2H5COOH+R1H=>.COOC2H5+H2    4.2E+06  2.1  4900.0  ! MAC 2284

! Ester metatesis

! Alkohol ene to dienes
C5H9OHZ+R1H=>H2+R2OH+C5H8Z2    9.0E+06  2.0  5000.0  ! ROH 2285
C5H9OHZ+R2OH=>H2O+R2OH+C5H8Z2    1.3E+09  1.3  700.0  ! ROH 2286
C5H9OHZ+R3O2H=>H2O2+R2OH+C5H8Z2    4.0E+11  0.0  15500.0  ! ROH 2287
C5H9OHZ+R4CH3=>CH4+R2OH+C5H8Z2    2.0E+11  0.0  9600.0  ! ROH 2288
C5H9OHZ+R11C2H5=>C2H6+R2OH+C5H8Z2    2.0E+11  0.0  11000.0  ! ROH 2289
C6H11OHZ+R1H=>H2+R2OH+C6H10Z2    9.0E+06  2.0  5000.0  ! ROH 2290
C6H11OHZ+R2OH=>H2O+R2OH+C6H10Z2    1.3E+09  1.3  700.0  ! ROH 2291
C6H11OHZ+R3O2H=>H2O2+R2OH+C6H10Z2    4.0E+11  0.0  15500.0  ! ROH 2292
C6H11OHZ+R4CH3=>CH4+R2OH+C6H10Z2    2.0E+11  0.0  9600.0  ! ROH 2293
C6H11OHZ+R11C2H5=>C2H6+R2OH+C6H10Z2    2.0E+11  0.0  11000.0  ! ROH 2294

! Diels Alder
C4H6Z2+C2H4Z=>C6H10#ZZ2    3.0E+10  0.0  27500.0  ! DA 2295
C5H8Z2+C2H4Z=>C7H12#ZZ2    3.0E+10  0.0  27500.0  ! DA 2297
C6H10Z2+C2H4Z=>C8H14#ZZ2    3.0E+10  0.0  27500.0  ! DA 2298

! Peracide radical metathesis
.COOOC2H5+C6H14O=>R27C6H13O+R2OH+CO2+R11C2H5    9.0E+12  0.0  17500.0  ! PER 2299
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.COOOC2H5+C5H12O=>R25C5H11O+R2OH+CO2+R11C2H5    9.0E+12  0.0  17500.0  ! PER 2300
.COOOC2H5+C7H16=>R21C7H15+R2OH+CO2+R11C2H5    9.0E+12  0.0  17500.0  ! PER 2301
.COOOC3H7+C6H14O=>R27C6H13O+R2OH+CO2+R4CH3+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2302
.COOOC3H7+C5H12O=>R25C5H11O+R2OH+CO2+R4CH3+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2303
.COOOC3H7+C7H16=>R21C7H15+R2OH+CO2+R4CH3+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2304
.COOOC4H9+C6H14O=>R27C6H13O+R2OH+CO2+R11C2H5+C2H4Z    9.0E+12  0.0  17500.0  ! PER 230
5
.COOOC4H9+C5H12O=>R25C5H11O+R2OH+CO2+R11C2H5+C2H4Z    9.0E+12  0.0  17500.0  ! PER 230
6
.COOOC4H9+C7H16=>R21C7H15+R2OH+CO2+R11C2H5+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2307
.COOOC6H13+C6H14O=>R27C6H13O+R2OH+CO2+R11C2H5+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 2
308
.COOOC6H13+C5H12O=>R25C5H11O+R2OH+CO2+R11C2H5+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 2
309
.COOOC6H13+C7H16=>R21C7H15+R2OH+CO2+R11C2H5+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 231
0
.COOOC5H11+C6H14O=>R27C6H13O+R2OH+CO2+R4CH3+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 231
1
.COOOC5H11+C5H12O=>R25C5H11O+R2OH+CO2+R4CH3+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 231
2
.COOOC5H11+C7H16=>R21C7H15+R2OH+CO2+R4CH3+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 2313
.COOOC2H5=>C2H4Z+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2314
.COOOC3H7=>C3H6Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2315
.COOOC4H9=>C4H8Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2316
.COOOC6H13=>C6H12Z+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2317
.COOOC5H11=>C5H10Z+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2318

! Keto radicals to products of the base and :CO
.COC2H5=>B2CO+R11C2H5    2.0E+13  0.0  28700.0  ! COR 2319
.COC3H7=>B2CO+R4CH3+C2H4Z    2.0E+13  0.0  28700.0  ! COR 2320
.COC4H9=>B2CO+R11C2H5+C2H4Z    2.0E+13  0.0  28700.0  ! COR 2321
.COC6H13=>B2CO+R11C2H5+2C2H4Z    2.0E+13  0.0  28700.0  ! COR 2322
.COC5H11=>B2CO+R4CH3+2C2H4Z    2.0E+13  0.0  28700.0  ! COR 2323


! keto radicals addition to O2
.COC2H5+O2=>.COOOC2H5    2.4E+12  0.0  0.0  ! COR 2324
.COC3H7+O2=>.COOOC3H7    2.4E+12  0.0  0.0  ! COR 2325
.COC4H9+O2=>.COOOC4H9    2.4E+12  0.0  0.0  ! COR 2326
.COC6H13+O2=>.COOOC6H13    2.4E+12  0.0  0.0  ! COR 2327
.COC5H11+O2=>.COOOC5H11    2.4E+12  0.0  0.0  ! COR 2328

! Ester radicals reactions :

! .Y termination
.C3H5Y+R1H=>C3H6Y    1.0E+13  0.0  0.0  ! TER 2329
.C3H5Y+R2OH=>C3H5OHY    1.0E+13  0.0  0.0  ! TER 2330
.C3H5Y+R3O2H=>C3H5OOHY    5.0E+12  0.0  0.0  ! TER 2331
.C3H5Y+R4CH3=>C4H8Y    1.0E+13  0.0  0.0  ! TER 2332
.C3H5Y+R5CHO=>C3H5CHOY    1.0E+13  0.0  0.0  ! TER 2333
.C3H5Y+R6CH2OH=>C4H7OHY    1.0E+13  0.0  0.0  ! TER 2334
.C3H5Y+R11C2H5=>C5H10Z    1.0E+13  0.0  0.0  ! TER 2335
.C4H7Y+R1H=>C4H8Y    1.0E+13  0.0  0.0  ! TER 2336
.C4H7Y+R2OH=>C4H7OHY    1.0E+13  0.0  0.0  ! TER 2337
.C4H7Y+R3O2H=>C4H7OOHY    5.0E+12  0.0  0.0  ! TER 2338
.C4H7Y+R4CH3=>C5H10Z    1.0E+13  0.0  0.0  ! TER 2339
.C4H7Y+R5CHO=>C4H7CHOY    1.0E+13  0.0  0.0  ! TER 2340
.C4H7Y+R6CH2OH=>C5H9OHZ    1.0E+13  0.0  0.0  ! TER 2341
.C4H7Y+R11C2H5=>C6H12Z    1.0E+13  0.0  0.0  ! TER 2342
.C3H5Y+.C3H5Y=>C6H10Y2    1.0E+13  0.0  0.0  ! TER 2350
.C3H5Y+.C4H7Y=>C7H12Y2    1.0E+13  0.0  0.0  ! TER 2351
.C3H5Y+.C5H9Y=>C8H14Y2    1.0E+13  0.0  0.0  ! TER 2352
.C4H7Y+.C4H7Y=>C8H14Y2    1.0E+13  0.0  0.0  ! TER 2353
.C4H7Y+.C5H9Y=>C9H16Y2    1.0E+13  0.0  0.0  ! TER 2354
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! Pascal C0 C2 lumped data base

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


!REACTIONS DE H2!
H2+M=R1H+R1H+M                2.2E14          0.     95.7E3 !(1,-1)<BAULCH94>!

!REACTIONS DE B3C!
B3C+H2=B4CH+R1H               4.0E14      0.     23.3E3 !(2,-2)<DEAN91NIST>!

!REACTIONS DE B6CH2!
B6CH2+M=B5CH2+M               6.0E12          0.         0. !(3,-3)<BAULCH94AVERAGE>!
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            1.0E16      0.      90.4E3 !(8,-8)<BAULCH94>!
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)       3.6E13      0.         0.  !(14,-14)<BAULCH94>!
                     LOW     /1.3E41     -7.      3.0E3/
                     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!
CH4(+M)=R4CH3+R1H(+M)          2.4E16      0.    104.5E3 !(17,-17)<BAULCH94>!
                     LOW     /4.5E17      0.     90.5E3/
                     TROE    /1.     1.     1350.     7830./
CH4+R1H=R4CH3+H2               1.3E4       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=R9C2H+R1H                 2.6E15      0.    123.9E3 !(24,-24)<TSANG86>!
C2H2+R1H=R9C2H+H2              6.6E13      0.     27.7E3 !(25,-25)<BAULCH94>!

!REACTIONS DE R10C2H3D!
R10C2H3V(+M)=C2H2+R1H(+M)      2.0E14       0.     40.0E3 !(26,-26)<BAULCH94>!
                     LOW     /4.1E41     -7.5    45.3E3/
                     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>!
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!REACTIONS DE C2H4Z!
C2H4Z+M=C2H2+H2+M              3.5E16      0.     71.3E3 !(33,-33)<BAULCH94>!
C2H4Z+M=R10C2H3V+R1H+M         2.6E17      0.     96.2E3 !(34,-34)<BAULCH94>!
C2H4Z+R1H=R10C2H3V+H2          5.4E14      0      14.8E3 !(35,-35)<BAULCH94>!
C2H4Z+R4CH3=CH4+R10C2H3V       4.1E12      0.     11.1E3 !(36,-36)<BAULCH94>!

!REACTIONS DE R11C2H5!
R11C2H5(+M)=C2H4Z+R1H(+M)       8.2E13      0.     40.0E3 !(37,-37)<BAULCH94>!
                    LOW     /1.0E18      0.     33.3E3/
                    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)<MURRELL86NIST>!
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)<DEAN87NIST>!
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=R12CHCOZ+R1H           6.5E3       2.8     0.5E3 !(64,-64)<DAGAUT91>!
B1O+C2H2=B5CH2+B2CO             1.5E4       2.8     0.5E3 !(65,-65)<DAGAUT91>!
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!
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R2OH+M=B1O+R1H+M                2.4E15      0.     99.0E3 !(77,-77><TSANG86>!
R2OH+R1H+M=H2O+M                2.4E22     -2.0        0. !(78,-78)<BAULCH94>!
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            7.2E12      0.      2.7E3 !(84,-84)<BAULCH94>!
R2OH+R4CH3=B6CH2+H2O            7.2E13      0.      2.7E3 !(84,-84)<BAULCH94corrigeLeed
s>
R2OH+R4CH3(+M)=CH3OH(+M)        6.0E13      0.         0. !(85,-85)<BAULCH94>!
!valeur de k0 dans Ar (1000-2000 K)
                    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             1.4E4       2.68   12.0E3 !(92,-92)<TSANG86>!
R2OH+C2H2=CH2COZ+R1H            2.2E-4      4.5    -1.0E3 !(93,-93)<DAGAUT91>!
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>!
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                6.2E14      0.      3.0E3 !(106,-106)<TSANG86>!
B2CO+R2OH=CO2+R1H               6.3E6       1.5    -0.5E3 !(107,-107)<BAULCH94>!

!REACTIONS DE R5CHO!
R5CHO+M=R1H+B2CO+M              1.6E14      0.     15.7E3 !(108,-108)<BAULCH94>!
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>!
R5CHO+CH4=R4CH3+HCHO            7.3E3       2.85   22.4E3 !(115,-115)<TSANG86>!
R5CHO+R9C2H=C2H2+B2CO           6.0E13      0.         0. !(116,-116)<TSANG86>!
R5CHO+R10C2H3V=C2H4Z+B2CO       9.0E13      0.         0. !(117,-117)<TSANG86>!
R5CHO+C2H4Z=R10C2H3V+HCHO       9.0E10      0.      5.4E3 !(118,-118)<LESCLAUX86NIST>!
R5CHO+R11C2H5=C2H6+B2CO         1.2E14      0.         0. !(119,-119)<TSANG86>!
R5CHO+C2H6=R11C2H5+HCHO         4.7E4       2.72   18.2E3 !(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!
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HCHO+M=R5CHO+R1H+M              4.9E35     -5.54    96.3E3 !(125,-125)<BAULCH94>!
HCHO+M=B2CO+H2+M                1.1E36     -5.54    96.3E3 !(126,-126)<BAULCH94>!
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             3.4E9       1.18    -0.4E3 !(131,-131)<BAULCH94>!

!REACTIONS DE R7CH3O!
R7CH3O+M=HCHO+R1H+M             5.4E13      0.      13.4E3 !(132,-132)<BAULCH94>!
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+R4CH3=CH3OCH3           1.2E13      0.         0. !<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>!
!R7CH3O+R7CH3O=CH3OOCH3         1.8E12      0.         0. !<TSANG86>!


!REACTIONS DE R6CH2OH!
R6CH2OH+M=R1H+HCHO+M            4.5E25     -2.5     34.2E3 !(149,-149)<TSANG87>!
R6CH2OH+R1H=R4CH3+R2OH          9.6E13      0.         0. !(150,-150)<TSANG87>!
R6CH2OH+R1H=HCHO+H2             6.0E12      0.         0. !(151,-151)<TSANG87>!
R6CH2OH+H2=CH3OH+R1H            6.7E5       2.      13.4E3 !(152,-152)<TSANG87>!
R6CH2OH+B6CH2=CH3CHO+R1H        1.8E13      0.         0. !(153,-153)<TSANG87>!
R6CH2OH+B5CH2=C2H4Z+R2OH        2.4E13      0.         0. !(154,-154)<TSANG87>!
R6CH2OH+B5CH2=R4CH3+HCHO        1.2E12      0.         0. !(155,-155)<TSANG87>!
R6CH2OH+R4CH3=C2H5OH            1.2E13      0.         0. !(156,-156)<TSANG87>!
R6CH2OH+R4CH3=CH4+HCHO          2.4E12      0.         0. !(157,-157)<TSANG87>!
R6CH2OH+CH4=CH3OH+R4CH3         21.7        3.1     16.2E3 !(158,-158)<TSANG87>!
R6CH2OH+R9C2H=C2H2+HCHO        4.8E13      0.          0. !(159,-159)<TSANG87>!
!la constante de vitesse du processus 159 est globalisee!
!R6CH2OH+R9C2H=C3H3+R2OH       1.2E13      0.          0. !(159a,-159a)<TSANG87>!
!R6CH2OH+R9C2H=C2H2+HCHO       3.6E13      0.          0. !(159b,-159b)<TSANG87>!
R6CH2OH+C2H2=R10C2H3V+HCHO      7.2E11      0.       9.0E3 !(160,-160)<TSANG87>!
R6CH2OH+R10C2H3V=C2H4Z+HCHO     4.2E13      0.         0. !(161,-161)<TSANG87>!
!La constante de vitesse  du processus 161 est globalisee!
R6CH2OH+R11C2H5=C2H4Z+CH3OH     2.4E12      0.         0. !(162,-162)<TSANG87>!
R6CH2OH+R11C2H5=C2H6+HCHO       2.4E12      0.         0. !(163,-163)<TSANG87>!
R6CH2OH+C2H6=CH3OH+R11C2H5      199.        3.      14.0E3 !(164,-164)<TSANG87>!
R6CH2OH+B1O=HCHO+R2OH           4.2E13      0.         0. !(165,-165)<TSANG87>!
R6CH2OH+R2OH=H2O+HCHO           2.4E13      0.         0. !(166,-166)<TSANG87>!
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!
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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)<GROTHEER81NIST>!
CH3OH+B1O=R7CH3O+R2OH          1.0E13      0.      4.7E3 !(183,-183)<WARNATZ84>!
CH3OH+R2OH=R7CH3O+H2O          1.0E13      0.      1.7E3 !(184,-184)<WARNATZ84>!
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. !(187,-187)<BAULCH94>!
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          4.1E15      0.     59.3E3 !(192,-192)<DAGAUT91>!
CH2COZ+M=R12CHCOZ+R1H+M        2.7E17      0.     87.0E3 !(193,-193)<FRANK86NIST>!
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>!

!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>!
! modif le 11 mai 1995 pour le butane (FBL)
! CH3CHO+R4CH3=R14CH3CO+CH4      1.2E11      0.       2.5E3!(216,-216)<COX90*>!
CH3CHO+R4CH3=R14CH3CO+CH4       2.0E-6      5.6      2.5E3!(216,-216)<COX90*>!
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)<SCHUCHMANN70NIS
T>!
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!* n=0 was assumed
!REACTIONS DE C2H4O#!
C2H4O#3=CH4+B2CO                  1.2E13      0.      57.2E3!(223,-223)<LIFSHITZ83NIS
T>!
C2H4O#3=CH3CHO                    7.3E13      0.      57.2E3!(224,-224)<LIFSHITZ83NIS
T>!
C2H4O#3=R4CH3+R5CHO               3.6E13      0.      57.2E3!(225,-225)<LIFSHITZ83NIS
T>!
C2H4O#3+R1H=H2+R13CH2CHO          2.0E13      0.       8.3E3!(226,-226)<LIFSHITZ83NIS
T*>!
C2H4O#3+R1H=H2O+R10C2H3V          5.0E9       0.       5.0E3!(227,-227)<LIFSHITZ83NIS
T>!
C2H4O#3+R1H=C2H4Z+R2OH            9.5E10      0.       5.0E3!(228,-228)<LIFSHITZ83NIS
T>!
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!
!(C2H5OH+H, O, OH =products          no enough data)
C2H5OH+R1H=H2+R1H+CH3CHO       4.4E+12    0.     4.57E+3 !<ADERS73NIST>!
C2H5OH+B1O=R2OH+R1H+CH3CHO     3.4E+13    0.      5.5E+3 !<comme CH3OH>!
C2H5OH+R2OH=H2O+R1H+CH3CHO     2.6E+06    2.     -1370.0 !<Atkinson>!
C2H5OH+R4CH3=CH4+R1H+CH3CHO    4.0E+11    0.     9.69E+3 !<GRAY68NIST>!
C2H5OH+R1H=H2+R2OH+C2H4Z       4.4E+12    0.     8.57E+3 !<+4kcal>!
C2H5OH+B1O=R2OH+R2OH+C2H4Z     3.4E+13    0.      9.5E+3 !<+4kcal>!
C2H5OH+R2OH=H2O+R2OH+C2H4Z     2.7E+06    2.0      450.0 !<Atkinson>!
C2H5OH+R4CH3=CH4+R2OH+C2H4Z    4.0E+11    0.    13.69E+3 !<+4kcal>!

!REACTIONS DE O2!
O2+M=B1O+B1O+M                 1.8E18     -1.    118.1E3 !(244,-244)<TSANG86>!
O2+R1H=R2OH+B1O                9.8E13      0.     14.8E3 !(245,-245)<BAULCH94>!
O2+R1H+M=R3O2H+M               6.2E17     -0.8        0. !(246,-246)<BAULCH94>!
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              2.0E13      0.         0. !(249,-249)<DAGAUT91>!
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>!
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O2+R4CH3=HCHO+R2OH              3.0E30     -4.69   36.6E3 !(259,-259)<DAGAUT91>!
O2+CH4=R4CH3+R3O2H              4.0E13      0.     56.7E3 !(260,-260)<BAULCH94>!
O2+R9C2H=B2CO+R5CHO            2.4E12      0.        0. !(261,-261)<TSANG86>!
O2+R9C2H=R12CHCOZ+B1O          6.0E11      0.        0. !(262,-262)<TSANG86>!
O2+C2H2=R9C2H+R3O2H            1.2E13      0.     74.5E3 !(263,-263)<TSANG86>!
O2+C2H2=R12CHCOZ+R2OH           2.0E8       1.5    30.1E3 !(264,-264)<DAGAUT91>!
O2+R10C2H3V=C2H2+R3O2H          1.2E11      0.        0. !(265,-265)<TSANG86>!
O2+R10C2H3V=HCHO+R5CHO          3.0E12      0.     -0.3E3 !(266,-266)<DAGAUT91>!
O2+C2H4Z=R10C2H3V+R3O2H         4.2E13      0.     57.4E3 !(267,-267)<TSANG86>!
O2+R11C2H5=R17C2H5OO            2.2E10      0.77   -0.6E3 !(268,-268)<WAGNER90>!
O2+R11C2H5=C2H4Z+R3O2H          8.4E11      0.      3.9E3 !(269,-269)<TSANG86>!
O2+R11C2H5=R15C2H5O+B1O         1.2E13     -0.2    27.9E3 !(270,-270)<BOZZELLI90NIST>!
O2+R11C2H5=CH3CHO+R2OH          6.0E10      0.      6.9E3 !(271,-271)<TSANG86>!
O2+C2H6=R11C2H5+R3O2H           6.0E13      0.     51.7E3 !(272,-272)<BAULCH94>!
O2+R2OH=R3O2H+B1O               2.2E13      0.     52.5E3 !(273,-273)<TSANG86>!
O2+B2CO=CO2+B1O                 2.5E12      0.     47.7E3 !(274,-274)<TSANG86>!
O2+R5CHO=B2CO+R3O2H             5.1E13      0.      1.7E3 !(275,-275)<TSANG86>!
O2+HCHO=R5CHO+R3O2H             2.0E13      0.     38.8E3 !(276,-276)<TSANG86)!


O2+R7CH3O=HCHO+R3O2H            2.2E10      0.      1.7E3 !(277,-277)<BAULCH94>!
O2+R6CH2OH=HCHO+R3O2H           1.2E12      0.        0. !(278,-278)<TSANG87>!
O2+CH3OH=R6CH2OH+R3O2H          2.0E13      0.     44.9E3 !(279,-279)<TSANG87>!
O2+R12CHCOZ=>B2CO+B2CO+R2OH     1.5E12      0.      2.5E3 !(280)     <DAGAUT91>!
O2+CH2COZ=HCHO+CO2              1.0E8       0.        0. !(281,-281)<DAGAUT91>!
O2+R14CH3CO=R18CH3COOO          2.4E12      0.        0. !(282,-282)<COX90>!
O2+R13CH2CHO=>HCHO+R2OH+B2CO    5.9E9       0.     -1.4E3 !(283)     <COX90>!
O2+R13CH2CHO=CH2COZ+R3O2H       1.0E10      0.     -1.4E3 !(284,-284)<COX90>!
O2+CH3CHO=R14CH3CO+R3O2H        5.0E13      0.     36.4E3 !(285,-285)<COX90>!
! ajout demande par Laetitia le 25 Avril 95
O2+CH3CHO=R13CH2CHO+R3O2H       1.0E13      0.5    46.0E3 !(285',-285)<Ranzi94>!
O2+C2H4O#3=R3O2H+R13CH2CHO      5.0E13      0.     48.0E3 !(286,-286)<RANZI94>!
O2+R15C2H5O=CH3CHO+R3O2H        6.0E10      0.      1.7E3 !(287,-287)<BAULCH94>!

!REACTIONS DE R3O2H!
R3O2H+R1H=H2+O2                  4.3E13      0.      1.4E3 !(288,-288)<BAULCH94>!
R3O2H+R1H=2R2OH                  1.7E14      0.      0.9E3 !(289,-289)<BAULCH94>!
R3O2H+R1H=H2O+B1O                3.0E13      0.      1.7E3 !(290,-290)<BAULCH94>!
R3O2H+B6CH2=HCHO+R2OH            3.0E13      0.        0. !(291,-291)<TSANG86>!
R3O2H+B5CH2=HCHO+R2OH            1.8E13      0.        0. !(292,-292)<TSANG86>!
R3O2H+R4CH3=R7CH3O+R2OH          1.8E13      0.        0. !(293,-293)<BAULCH94>!
R3O2H+CH4=R4CH3+H2O2             9.0E12      0.     24.6E3 !(294,-294)<BAULCH94>!
R3O2H+R9C2H=R12CHCOZ+R2OH       1.8E13      0.        0. !(295,-295)<TSANG86>!
R3O2H+C2H2=CH2COZ+R2OH           6.0E9       0.      8.0E3 !(296,-296)<TSANG86>!
R3O2H+R10C2H3V=>R2OH+R4CH3+B2CO 3.0E13      0.        0. !(297)     <TSANG86>!
R3O2H+C2H4Z=CH3CHO+R2OH          6.0E9       0.      7.9E3 !(298,-298)<TSANG86>!
R3O2H+C2H4Z=C2H4O#3+R2OH         2.2E12      0.     17.2E3 !(299,-299)<BAULCH94>!
R3O2H+R11C2H5=>R4CH3+HCHO+R2OH  2.4E13      0.        0. !(300)     <TSANG86>!
R3O2H+R11C2H5=C2H4Z+H2O2         3.0E11      0.        0. !(301,-301)<TSANG86>!
R3O2H+C2H6=R11C2H5+H2O2          1.3E13      0.     20.4E3 !(302,-302)<BAULCH94>!
R3O2H+R2OH=H2O+O2                2.9E13      0.     -0.5E3 !(303,-303)<BAULCH94>!
R3O2H+B2CO=CO2+R2OH              1.5E14      0.     23.6E3 !(304,-304)<TSANG86>!
R3O2H+R5CHO=>R2OH+R1H+CO2        3.0E13      0.        0. !(305)     <TSANG86>!
R3O2H+HCHO=R5CHO+H2O2            3.0E12      0.     13.0E3 !(306,-306)<BAULCH94>!
R3O2H+R7CH3O=HCHO+H2O2           3.0E11      0.        0. !(307,-307)<TSANG86>!
R3O2H+R6CH2OH=HCHO+H2O2          1.2E13      0.        0. !(308,-308)<TSANG87>!
R3O2H+CH3OH=R6CH2OH+H2O2         9.6E10      0.     12.6E3 !(309,-309)<TSANG87>!
R3O2H+R14CH3CO=>R4CH3+CO2+R2OH  3.0E13      0.        0. !(310)<TSANG86>!
R3O2H+CH3CHO=R14CH3CO+H2O2       1.0E12      0.     10.0E3 !(311,-311)<CAVANAGH90>!
R3O2H+C2H4O#3=H2O2+R13CH2CHO     1.6E12      0.     15.0E3 !(312,-312)<RANZI94>
!
!       modification le 11 Avril 1995 :
!       BAULCH : valeur valable a T > 850 K :
!       R3O2H+R3O2H=H2O2+O2             1.9E12      0.      1.5E3 !(313,-313)<BAULCH92
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>!
!       valeur valable a T < 850 K :
!       R3O2H+R3O2H=H2O2+O2              2.0E12      0.      0.0E0 !(313,-313)<RANZI 94
>!
!       valeur de Baulch 94 :  modif du 11 mai 1995.
!       R3O2H+R3O2H=H2O2+O2              1.3E11      0.      -1.7E3 !(313,-313)<BAULCH
94>!
!       valeur de Tsang 86 :  modif du 2 avril 1996.
!       R3O2H+R3O2H=H2O2+O2              1.8E12      0.      0. !(313,-313)<TSANG 86>!
!       modification janvier 1997 valeurs pour tout T
R3O2H+R3O2H=H2O2+O2              1.3E11      0.      -1.63E3 !(313,-313)<BAULCH 94>!
     DUPLICATE
R3O2H+R3O2H=H2O2+O2              4.2E14      0.      11.98E3 !(313,-313)<BAULCH 94>!
     DUPLICATE

!REACTIONS DE H2O2!
H2O2(+M)=R2OH+R2OH(+M)          3.0E14      0.     48.3E3 !(314,-314)<BAULCH94>!
                    LOW     /1.2E17      0.     45.3E3/
                    TROE    /1.0         1.0    1.0E8/
H2O2+R1H=H2+R3O2H               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+R3O2H       1.2E10      0.     -0.6E3 !(318,-318)<TSANG86>!
H2O2+B1O=R2OH+R3O2H             6.6E11      0.      4.0E3 !(319,-319)<BAULCH94>!
H2O2+R2OH=H2O+R3O2H             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=CH3O2H+R1H             3.0E13      0.     26.0E3 !(324,-324)<TSANG86>!
R8CH3OO+B6CH2=HCHO+R7CH3O         1.8E13      0.         0. !(325,-325)<TSANG86>!
R8CH3OO+B5CH2=HCHO+R7CH3O         1.8E13      0.         0. !(326,-326)<TSANG86>!
R8CH3OO+R4CH3=R7CH3O+R7CH3O       5.0E12      0.     -1.4E3 !(327,-327)<CAVANAGH90>!
R8CH3OO+CH4=CH3O2H+R4CH3          1.8E11      0.     18.5E3 !(328,-328)<TSANG86>!
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ    2.4E13      0.         0. !(329,-329)<TSANG86>!
R8CH3OO+C2H2=CH3O2H+R9C2H        5.6E11      0.     24.5E3 !(330,-330)<RANZI94>!
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 2.4E13      0.         0. !(331,-331)<TSANG86*>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3      1.1E15      0.     20.0E3 !(332,-332)<NIKISHA81/MOSH
KINA80NIST>!
R8CH3OO+C2H4Z=CH3O2H+R10C2H3V     3.9E12      0.     24.5E3 !(333,-333)<RANZI94>!
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O  2.4E13      0.         0. !(334,-334)<TSANG86>!
R8CH3OO+C2H6=CH3O2H+R11C2H5       2.9E11      0.     14.9E3 !(335,-335)<TSANG86>!
R8CH3OO+B1O=R7CH3O+O2             3.6E13      0.         0. !(336,-336)<TSANG86>!
R8CH3OO+R2OH=CH3OH+O2             6.0E13      0.         0. !(337,-337)<TSANG86>!
R8CH3OO+R2OH=R7CH3O+R3O2H         3.0E12      0.         0. !(338,-338)<RANZI94>!
R8CH3OO+B2CO=R7CH3O+CO2           1.0E14      0.     24.0E3 !(339,-339)<RANZI94>!
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2     3.0E13      0.         0. !(340)     <TSANG86>!
R8CH3OO+HCHO=CH3O2H+R5CHO         1.0E12      0.     12.1E3 !(341,-341)<CAVANAGH90>!
R8CH3OO+R7CH3O=HCHO+CH3O2H        3.0E11      0.         0. !(342,-342)<TSANG86>!
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO 1.2E13      0.         0. !(343)<TSANG87>!
R8CH3OO+CH3OH=CH3O2H+R6CH2OH      1.8E12      0.     13.7E3 !(344,-344)<TSANG87>!
R8CH3OO+CH3OH=CH3O2H+R7CH3O       2.8E11      0.     18.8E3 !(345,-345)<RANZI94>!
R8CH3OO+CH2COZ=CH3O2H+R12CHCOZ    1.7E12      0.     27.0E3 !(346,-346)<RANZI94>!
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O 2.4E13      0.         0. !(347,-347)<TSANG86>!
R8CH3OO+CH3CHO=CH3O2H+R14CH3CO    1.0E12      0.     12.1E3 !(348,-348)<CAVANAGH90>!
R8CH3OO+CH3CHO=CH3O2H+R13CH2CHO   1.7E12      0.     19.2E3 !(349,-349)<RANZI94>!
R8CH3OO+C2H4O#3=CH3O2H+R13CH2CHO  2.2E12      0.     16.0E3 !(350,-350)<RANZI94>!
R8CH3OO+R3O2H=CH3O2H+O2           2.5E11      0.     -1.6E3 !(351,-351)<BAULCH94>!
R8CH3OO+R3O2H=>O2+HCHO+H2O        5.0E10      0.         0. !(352)<RANZI94>!
R8CH3OO+H2O2=CH3O2H+R3O2H         2.4E12      0.      9.9E3 !(353,-353)<TSANG86>!
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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>!

!REACTIONS DE CH3O2H!
CH3O2H=R7CH3O+R2OH               6.0E14      0.     42.3E3 !(356,-356)<BAULCH94>!
CH3O2H+B1O=R8CH3OO+R2OH          2.0E13      0.      4.8E3 !(357,-357)<BAULCH94average
>!
CH3O2H+R2OH=H2O+R8CH3OO          1.8E12      0.    -0.37E3 !(358,-358)<BAULCH94average
>!
CH3O2H+R7CH3O=>CH3OH+R2OH+HCHO   1.5E11      0.      6.5E3 !(359)<RANZI94>!

!REACTIONS DE R17C2H5OO!
R17C2H5OO=R16C2H4O2H             4.2E12      0.     36.9E3 !(360,-360)<HUGHES93>!
R17C2H5OO+H2=C2H5O2H+R1H         7.9E12      0.     21.0E3 !(361,-361)<RANZI94>!
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O  2.0E12      0.     -1.2E3 !(362,-362)<RANZI94>!
R17C2H5OO+CH4=C2H5O2H+R4CH3      3.9E12      0.     24.0E3 !(363,-363)<RANZI94>!
R17C2H5OO+C2H2=C2H5O2H+R9C2H    5.6E11      0.     24.4E3 !(364,-364)<RANZI94>!
R17C2H5OO+C2H4Z=C2H5O2H+R10C2H3V 3.9E12      0.     24.4E3 !(365,-365)<RANZI94>!
R17C2H5OO+C2H4Z=R15C2H5O+C2H4O#3  2.3E16      0.     21.9E3 !(366,-366)<MOSHKINA80NIST
>!
R17C2H5OO+C2H6=C2H5O2H+R11C2H5   5.1E12      0.     19.5E3 !(367,-367)<RANZI94>!
R17C2H5OO+H2O=C2H5O2H+R2OH       5.6E12      0.     30.6E3 !(368,-368)<RANZI94>!
R17C2H5OO+B2CO=CO2+R15C2H5O      1.0E14      0.     24.0E3 !(369,-369)<RANZI94>!
R17C2H5OO+HCHO=C2H5O2H+R5CHO     4.5E12      0.     14.4E3 !(370,-370)<RANZI94>!
R17C2H5OO+CH3OH=C2H5O2H+R7CH3O   2.8E11      0.     18.4E3 !(371,-371)<RANZI94>!
R17C2H5OO+CH3OH=C2H5O2H+R6CH2OH  2.8E12      0.     19.5E3 !(372,-372)<RANZI94>!
R17C2H5OO+CH2COZ=C2H5O2H+R12CHCOZ  1.7E12      0.     24.4E3 !(373,-373)<RANZI94>!
R17C2H5OO+CH3CHO=C2H5O2H+R14CH3CO  3.9E12      0.     14.4E3 !(374,-374)<RANZI94>!
R17C2H5OO+CH3CHO=C2H5O2H+R13CH2CHO 1.7E12      0.     19.5E3 !(375,-375)<RANZI94>!
R17C2H5OO+C2H4O#3=C2H5O2H+R13CH2CHO 2.2E12      0.     16.3E3 !(376,-376)<RANZI94>!
R17C2H5OO+R3O2H=O2+C2H5O2H       3.9E11      0.     -1.3E3 !(377,-377)<BAULCH89>!
!Rate constant measured between 240 and 380K!
R17C2H5OO+H2O2=C2H5O2H+R3O2H     4.5E11      0.     10.8E3 !(378,-378)<RANZI94>!
R17C2H5OO+R8CH3OO=>R15C2H5O+R7CH3O+O2  2.0E11      0.         0. !(379)<RANZI94>!
R17C2H5OO+CH3O2H=C2H5O2H+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)<LIGHTFOOT
92>!

!REACTIONS DE R16C2H4O2H!
R16C2H4O2H=C2H4O#3+R2OH       1.5E11      0.     20.0E3 !(383,-383)<RANZI94>!
R16C2H4O2H=R6CH2OH+HCHO      2.5E13      0.     27.5E3 !(384,-384)<RANZI94>!
R16C2H4O2H=C2H4Z+R3O2H       2.0E13      0.     23.5E3 !(385,-385)<RANZI94>!

!REACTIONS DE C2H5O2H
C2H5O2H=R15C2H5O+R2OH        4.0E15      0.     42.9E3 !(386,-386)<BAULCH94>!
C2H5O2H+R1H=>CH3CHO+R2OH+H2  3.2E13      0.      7.7E3 !(387)<RANZI94>!
C2H5O2H+R4CH3=>CH3CHO+R2OH+CH4 5.7E11      0.      8.7E3 !(388)<RANZI94>!
C2H5O2H+R9C2H=>CH3CHO+R2OH+C2H2 6.0E11      0.      9.2E3 !(389)<RANZI94>!
C2H5O2H+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12      0.      8.7E3 !(390)<RANZI94>!
C2H5O2H+R11C2H5=>CH3CHO+R2OH+C2H6 3.4E11      0.     11.4E3 !(391)<RANZI94>!
C2H5O2H+R2OH=>CH3CHO+R2OH+H2O    5.9E12      0.      0.9E3 !(392)<RANZI94>!
C2H5O2H+R5CHO=>CH3CHO+R2OH+HCHO  1.8E12      0.     16.7E3 !(393)<RANZI94>!
C2H5O2H+R7CH3O=>CH3CHO+R2OH+CH3OH  6.3E11      0.      5.5E3 !(394)<RANZI94>!
C2H5O2H+R6CH2OH=>CH3CHO+R2OH+CH3OH  4.2E11      0.     13.6E3 !(395)<RANZI94>!
C2H5O2H+R14CH3CO=>2CH3CHO+R2OH    2.0E12      0.     18.5E3 !(396)<RANZI94>!
C2H5O2H+R13CH2CHO=>2CH3CHO+R2OH   3.4E11      0.     15.7E3 !(397)<RANZI94>!
C2H5O2H+R3O2H=>CH3CHO+R2OH+H2O2  8.0E11      0.     16.2E3 !(398)<RANZI94>!
C2H5O2H+R8CH3OO=>CH3CHO+R2OH+CH3O2H   1.1E12      0.     16.7E3 !(399)<RANZI94>!
C2H5O2H+R17C2H5OO=>CH3CHO+R2OH+C2H5O2H   1.1E12      0.     16.7E3 !(400)<RANZI94>!

!REACTIONS DE R18CH3COOO!
R18CH3COOO+C2H4O#3=CH3COO2H+R13CH2CHO  1.0E12      0.      9.3E3 !(401,-402)<RANZI94>!
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R18CH3COOO+R3O2H=CH3COO2H+O2        5.5E10      0.     -2.6E3 !(402,-402)<COX90>!
R18CH3COOO+C2H5O2H=CH3COO2H+R17C2H5OO   5.0E11      0.      9.2E3 !(403,-403)<RANZI94>
!
R18CH3COOO+C2H5O2H=>CH3CHO+R2OH+CH3COO2H  5.0E11      0.      9.2E3 !(404)<RANZI94>!
R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2  1.7E12      0.     -1.0E3 !(405)<CAVANAGH90>!

!REACTIONS DE CH3COO2H!
CH3COO2H=>R4CH3+CO2+R2OH          1.0E16      0.     40.0E3 !(406)<CAVANAGH90>!

!REACTIONS PRODUISANT DES C2+
C2H4Z+R4CH3=>R19C3H7      2.1E11    0.     7.35E3  !(407)<BAULCH94>!
R11C2H5+C2H4Z=>R20C4H9    1.1E11    0.     7.3E3   !(408)<BAULCH94>!

!REACTIONS DONNANT DES MOLECULES EN C3-C4!

!REACTIONS DE R9C2H!
!R9C2H+R9C2H=>C4H2                 1.8E13      0.         0. !(24,-24)<TSANG86>!

!REACTIONS DE C2H2!
!C2H2+B6CH2=>C3H4             1.7E14      0.         0. !(27,-27)<BAULCH94>!
!C2H2+B5CH2=>C3H4               3.5E12      0.         0. !(28,-28)<TSANG86>!
!C2H2+R4CH3=>C3H4+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>!
R10C2H3V+R10C2H3V=>C4H6Z2             9.6E12      0.         0. !(41,-41)<TSANG86>!

!REACTIONS DE C2H4!
!C2H4Z+B4CH=>C3H4+R1H             1.3E14      0.     -0.3E3 !(46,-46)<BAULCH94>!
C2H4Z+B6CH2=>C3H6Y            9.6E13      0.         0. !(47,-47)<BAULCH94>!
C2H4Z+B5CH2=>C3H6Y               3.2E12      0.      5.1E3 !(48,-48)<BAULCH94>!
!C2H4Z+R9C2H=>C4H4+R1H            1.2E13      0.         0. !(50,-50)<TSANG86>!
C2H4Z+R4CH3=>C3H6Y+R1H            6.6E11      0.        15.9E3  !<TSANG86>!
C2H4Z+R10C2H3V=>C4H6Z2+R1H           5.0E11      0.      7.3E3 !(51,-51)<TSANG86>!

!REACTIONS DE C2H5!
R11C2H5+B6CH2=>C3H6Y+R1H          9.0E12      0.         0. !(56,-56)<TSANG86>!
R11C2H5+R4CH3=>C3H8               3.4E13      0.         0. !(59,-59)<BAULCH94>!
R11C2H5+R10C2H3V=>C4H8Y             1.5E13      0.         0. !(61,-61)<TSANG86>!
R11C2H5+R11C2H5=>C4H10            1.1E13      0.         0. !(65,-65)<BAULCH94>!

!REACTIONS DE C2H6!
C2H6+B4CH=>C3H6Y+R1H              1.1E14      0.     -0.3E3 !(68,-68)<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!
!R7CH3O+R4CH3=>CH3OCH3            1.2E13      0.         0. !(159,-159)<TSANG86>!
!R7CH3O+R7CH3O=>CH3OOCH3          1.8E12      0.         0. !(172,-172)<TSANG86>!

!REACTIONS DE CH2OH!
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>!
!R14CH3CO+R5CHO=>CH3COCHO           1.8E13      0.         0. !(237,-237)<TSANG86>!
!R14CH3CO+R6CH2OH=>CH3COCH2OH          1.2E13      0.         0. !(241,-241)<TSANG87>
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!
!R14CH3CO+R14CH3CO=>CH3COCOCH3       1.2E13      0.     12.3E3 !(243,-243)<TSANG86>!

!REACTIONS DE CH3CHO!
CH3CHO+R14CH3CO=>C2H6CO+R5CHO            1.7E11      0.         0. !(254,-254)<GILL81>
!

END
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