```
!*****************************************************************************
*
!
!
!                      DEPARTEMENT DE CHIMIE PHYSIQUE DES REACTIONS
!
!                                   ENSIC-CNRS                                !
!                             1 RUE GRANDVILLE, BP 451
!
!                            54001 NANCY CEDEX - FRANCE
!
!
!
!*****************************************************************************
*
!
!
!                    COMPLETE MECHANISM FOR THE OXIDATION OF N-HEPTANE
 !
!                              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
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
C8H18
C5H10Y
C7H14Y
C6H12Z
C8H16Y
C3H5OOHY
C6H11OOHZ
C4H7OOHY
C5H9OOHZ
C7H13OOHY
C3H7CHO
C6H14CO
C4H9CHO
C6H13CHO
C7H15CHO
C2H4CHOOOH
C3H6CHOOOH
C6H13COOOH
C6H12CHOOOH
C7H14CHOOOH
C7H15COOOH
C2H5COOOH
C3H7COOOH
C4H8CHOOOH
C4H9COOOH
C4H10CO
C4H9OH
C4H9OOH
C3H7OOH
C5H12
C5H11OH
C5H12O
C4H10O
C6H14
C7H15OOH
C8H17OOH
C5H11OOH

! Secondary molecules :
C3H5OHY
C4H7OHY
C4H6YZ
C5H11CHO
C6H11OHY
C6H10YZ
C5H9OHZ
C5H8Z2
C7H13OHY
C7H12YZ
C3H7COOH
C2H5COOH
C3H5CHOY
C6H10Y2
C7H12Y2
C8H14Y2

C10H18Y2
C11H20Y2
C4H7CHOY
C9H16Y2
C12H22Y2
C5H9CHOY
C13H24Y2
C7H13CHOY
C8H15OHY
C9H18Y
C14H26Y2
C15H28Y2
C8H15OOHY
C8H15CHOY
C9H17OHY
C10H20Y
C16H30Y2

! Cyclic primary molecules :
C2H4O#3
C3H6O#3
C3H6O#4
C4H8O#3
C4H8O#4
C4H8O#5
C7H14O#3
C7H14O#4
C7H14O#5
C7H14O#6
C8H16O#4
C8H16O#5
C8H16O#6
C8H16O#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
C8H15O#4OOH
C8H15O#5OOH
C8H15O#6OOH
C8H15O#3OOH
C5H9O#3OOH
C5H9O#4OOH
C5H9O#5OOH
C5H9O#6OOH

! Cyclic secondary molecules :
C6H10#ZOOY
C4H#3OH10COYCOOH
C8H14#ZYZ
C7H12#ZZ2
C9H16#ZYZ
C2H3O#4COOOH
C3H5O#4COOOH
C3H5O#5COOOH

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C6H11O#4COOOH
C6H11O#5COOOH
C6H11O#6COOOH
C7H13O#4COOOH
C7H13O#5COOOH
C7H13O#6COOOH
C4H7O#4COOOH
C4H7O#5COOOH
C4H7O#6COOOH

! Free radicals :
RC6H13
R1C7H15
R2C7H15
R1H
R2OH
R3O2H
R4CH3
R5CHO
R6CH2OH
R7CH3O
R8CH3OO
R9C2H
R10C2H3V
R11C2H5
R12CHCOZ
R13CH2CHO
R14CH3CO
R15C2H5O
R16C2H4O2H
R17C2H5OO
R18CH3COOO
R19C3H7
R20C4H9
R21C7H15
R22C7H15
R23C7H15
R24C7H15
R25C8H17
R26C8H17
R27C8H17
R28C8H17
R29C3H7OO
R30C4H9OO
R31C7H15OO
R32C7H15OO
R33C7H15OO
R34C7H15OO
R35C5H11
R36C8H17OO
R37C4H9
R38C8H17OO
R39C8H17OO
R40C4H9
R41C8H17OO
R42C5H11
R43C3H6OOH
R44C3H6OOH
R45C4H8OOH
R46C4H8OOH
R47C4H8OOH
R48C7H14OOH
R49C7H14OOH
R50C7H14OOH
```

R51C7H14OOH
R52C7H14OOH
R53C7H14OOH
R54C7H14OOH
R55C7H14OOH
R56C7H14OOH
R57C7H14OOH
R58C7H14OOH
R59C7H14OOH
R60C7H14OOH
R61C7H14OOH
R62C7H14OOH
R63C7H14OOH
R64C7H14OOH
R65C7H14OOH
R66C5H11OO
R67C5H11
R68C8H16OOH
R69C8H16OOH
R70C8H16OOH
R71C8H16OOH
R72C4H9OO
R73C8H16OOH
R74C8H16OOH
R75C8H16OOH
R76C8H16OOH
R77C8H16OOH
R78C8H16OOH
R79C4H9OO
R80C8H16OOH
R81C8H16OOH
R82C8H16OOH
R83C8H16OOH
R84C5H11OO
R85C3H6OOOOH
R86C3H6OOOOH
R87C4H8OOOOH
R88C4H8OOOOH
R89C4H8OOOOH
R90C4H8OOH
R91C7H14OOOOH
R92C7H14OOOOH
R93C7H14OOOOH
R94C7H14OOH
R95C5H10OOH
R96C7H14OOOOH
R97C7H14OOOOH
R98C5H10OOH
R99C7H14OOOOH
R100C7H14OOOOH
R101C3H6OOH
R102C7H14OOOOH
R103C7H14OOH
R104C4H8OOH
R105C7H14OOOOH
R106C5H10OOH
R107C7H14OOOOH
R108C7H14OOH
R109C7H14OOOOH
R110C7H14OOOOH
R111C7H14OOOOH
R112C7H14OOH
R113C3H6OOH
R114C7H14OOOOH

R115C4H8OOH
R116C7H14OOOOH
R117C7H14OOH
R118C7H14OOH
R119C7H14OOOOH
R120C7H14OOOOH
R121C7H14OOH
R122C7H14OOOOH
R123C5H10OOH
R124C5H10OOH
R125C5H10OOH
R126C5H10OOH
R127C5H11OO
R128C8H16OOOOH
R129C8H16OOOOH
R130C8H16OOOOH
R131C8H16OOH
R132C4H8OOH
R133C8H16OOOOH
R134C5H10OOH
R135C4H8OOH
R136C8H16OOOOH
R137C8H16OOOOH
R138C5H10OOH
R139C8H16OOOOH
R140C4H8OOH
R141C8H16OOOOH
R142C8H16OOOOH
R143C8H16OOOOH
R144C4H8OOH
R145C8H16OOOOH
R146C8H16OOOOH
R147C8H16OOOOH
R148C8H16OOOOH
R149C8H16OOH
R150C3H5O4H2
R151C3H5O4H2
R152C3H6OOOOH
R153C3H5O4H2
R154C3H5O4H2
R155C4H7O4H2
R156C4H8OOOOH
R157C4H7O4H2
R158C4H7O4H2
R159C4H7O4H2
R160C4H7O4H2
R161C4H7O4H2
R162C4H8OOOOH
R163C4H7O4H2
R164C4H7O4H2
R165C4H8OOOOH
R166C7H13O4H2
R167C7H13O4H2
R168C7H13O4H2
R169C7H13O4H2
R170C7H13O4H2
R171C7H13O4H2
R172C7H13O4H2
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R182C5H10OOOOH
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R185C7H13O4H2
R186C7H13O4H2
R187C7H13O4H2
R188C7H13O4H2
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R190C7H13O4H2
R191C7H13O4H2
R192C7H13O4H2
R193C7H13O4H2
R194C5H10OOOOH
R195C7H13O4H2
R196C7H13O4H2
R197C7H13O4H2
R198C7H13O4H2
R199C7H13O4H2
R200C3H6OOOOH
R201C7H13O4H2
R202C7H13O4H2
R203C7H13O4H2
R204C7H13O4H2
R205C7H13O4H2
R206C7H14OOOOH
R207C4H9OO
R208C7H13O4H2
R209C7H13O4H2
R210C7H13O4H2
R211C7H13O4H2
R212C5H10OOOOH
R213C5H11OO
R214C5H10OOH
R215C7H13O4H2
R216C7H13O4H2
R217C7H13O4H2
R218C7H13O4H2
R219C7H14OOOOH
R220C7H13O4H2
R221C7H13O4H2
R222C7H13O4H2
R223C7H13O4H2
R224C7H13O4H2
R225C7H13O4H2
R226C7H14OOOOH
R227C3H7OO
R228C7H13O4H2
R229C7H13O4H2
R230C7H13O4H2
R231C7H13O4H2
R232C7H13O4H2
R233C7H13O4H2
R234C7H14OOOOH
R235C7H14OOOOH
R236C7H13O4H2
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R251C8H15O4H2
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R258C8H15O4H2
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R260C8H15O4H2
R261C8H15O4H2
R262C8H15O4H2
R263C8H15O4H2
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R269C8H15O4H2
R270C8H15O4H2
R271C5H10OOOOH
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R273C8H15O4H2
R274C8H15O4H2
R275C8H15O4H2
R276C8H15O4H2
R277C8H15O4H2
R278C8H15O4H2
R279C8H15O4H2
R280C5H10OOOOH
R281C8H15O4H2
R282C4H8OOOOH
R283C8H15O4H2
R284C8H15O4H2
R285C8H15O4H2
R286C4H8OOOOH
R287C8H15O4H2
R288C8H15O4H2
R289C8H15O4H2
R290C8H15O4H2
R291C8H15O4H2
R292C8H15O4H2
R293C8H15O4H2
R294C8H16OOOOH
R295C3H5O4H2
R296C4H7O4H2
R297C4H7O4H2
R298C4H7O4H2
R299C4H7O4H2
R300C4H7O4H2
R301C5H9O4H2
R302C5H9O4H2
R303C7H13O4H2
R304C7H13O4H2
R305C7H13O4H2
R306C5H9O4H2

R307C5H9O4H2
R308C5H9O4H2
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R310C5H10OOOOH
R311C5H10OOOOH
R312C5H10OOH
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R324C7H13O4H2
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R326C7H13O4H2
R327C4H8OOH
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R330C5H9O4H2
R331C5H9O4H2
R332C5H9O4H2
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R334C5H10OOOOH
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R336C7H13O4H2
R337C7H13O4H2
R338C7H13O4H2
R339C7H13O4H2
R340C5H9O4H2
R341C5H9O4H2
R342C5H9O4H2
R343C7H13O4H2
R344C7H13O4H2
R345C7H13O4H2
R346C7H13O4H2
R347C7H13O4H2
R348C3H7
R349C7H13O4H2
R350C7H13O4H2
R351C7H13O4H2
R352C7H13O4H2
R353C5H9O4H2
R354C7H13O4H2
R355C7H13O4H2
R356C7H13O4H2
R357C7H13O4H2
R358C5H9O4H2
R359C5H9O4H2
R360C5H9O4H2
R361C5H9O4H2
R362C5H9O4H2
R363C5H10OOOOH
R364C4H7O4H2
R365C5H9O4H2
R366C5H9O4H2
R367C8H15O4H2
R368C8H15O4H2
R369C8H15O4H2
R370C8H15O4H2

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R372C4H7O4H2
R373C4H7O4H2
R374C4H7O4H2
R375C5H9O4H2
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R377C4H7O4H2
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R379C8H15O4H2
R380C8H15O4H2
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R387C5H9O4H2
R388C5H10OOOOH
R389C4H8OOOOH
R390C5H9O4H2
R391C3H5O4H2
R392C4H7O4H2
R393C5H9O4H2
R394C5H9O4H2
R395C7H13O4H2
R396C7H13O4H2
R397C5H9O4H2
R398C7H13O4H2
R399C3H5O4H2
R400C4H7O4H2
R401C7H13O4H2
R402C7H13O4H2
R403C7H13O4H2
R404C7H13O4H2
R405C8H15O4H2
R406C8H15O4H2
R407C5H9O4H2
R408C5H9O4H2
R409C5H9O4H2
R410C4H7O4H2
R411C4H8OOOOH
R412C5H10OOOOH
R413C5H9O4H2
R414C3H6OOOOH
R415C4H7O4H2
R416C4H8OOH
R417C5H10OOH
R418C3H6OOH

! lumped Free radicals :
.C3H5Y
.C4H7Y
.COC2H5
.C5H9Y
.C7H13Y
.C8H15Y
.COC3H7
.COC4H9
.COC6H13
.COC7H15
.COC5H11
.COOC3H7
.COOC2H5
.COOOC2H5

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.COOOC3H7
.COOOC4H9
.COOOC6H13
.COOOC7H15
.COOOC5H11
! lumped Cyclic free radicals :
.C3H5O#4
.C4H7O#4
.C4H7O#5
.C7H13O#4
.C7H13O#5
.C7H13O#6
.C8H15O#4
.C8H15O#5
.C8H15O#6
.C5H9O#4
.C5H9O#5
.C5H9O#6
.OOC3H5O#4
.OOC4H7O#4
.OOC4H7O#5
.OOC7H13O#4
.OOC7H13O#5
.OOC7H13O#6
.OOC8H15O#4
.OOC8H15O#5
.OOC8H15O#6
.OOC5H9O#4
.OOC5H9O#5
.OOC5H9O#6
.C3H4O#4OOH
.C4H6O#4OOH
.C4H6O#5OOH
.C7H12O#4OOH
.C7H12O#5OOH
.C7H12O#6OOH
.C8H14O#4OOH
.C8H14O#5OOH
.C8H14O#6OOH
.C5H8O#4OOH
.C5H8O#5OOH
.C5H8O#6OOH
.OOC3H4O#4OOH
.OOC4H6O#4OOH
.OOC4H6O#5OOH
.OOC7H12O#4OOH
.OOC7H12O#5OOH
.OOC7H12O#6OOH
.OOC8H14O#4OOH
.OOC8H14O#5OOH
.OOC8H14O#6OOH
.OOC5H8O#4OOH
.OOC5H8O#5OOH
.OOC5H8O#6OOH

N2
HE
END

THERMO ALL
   300.000  1000.000  5000.000
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
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```
 9.68595E-09    1.20258E-12    1.37897E+03    3.16000E+01                    4
R1C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00     1
 1.20631E+01    4.40412E-02   -1.44547E-05    2.23337E-09   -1.33749E-13     2
-8.42961E+03   -3.29856E+01   -2.32443E-01    7.75812E-02   -3.87177E-05     3
-3.00145E-10    5.44697E-12   -5.29909E+03    2.99902E+01                    4
R2C7H15                C   7H  15O   0     G  0300.00   5000.00  1000.00     1
 1.37932E+01    4.26641E-02   -1.40081E-05    2.16542E-09   -1.29749E-13     2
-7.37213E+03   -4.41813E+01   -1.19307E+00    8.41335E-02   -4.47424E-05     3
-1.35861E-10    6.44865E-12   -3.61613E+03    3.23604E+01                    4
N2      Ranzi          0N   2C   0H   0O   0G  0300.00   5000.00  1000.00     1
 2.9266400E+00  1.4879770E-03 -5.6847603E-07  1.0097040E-10 -6.7533509E-15     2
-922.76760E+00  5.9805290E+00  3.2986770E+00  1.4082399E-03 -3.9632218E-06     3
 5.6415148E-09 -2.4448540E-12 -1020.9000E00   3.9503720E+00                   4
HE      Ranzi          0HE  2C   0H   0O   0G  0300.00   5000.00  1000.00     1
 3.1250000E+00 -1.4062505E-03  9.3750049E-07 -1.5625008E-10  0.0000000E+00     2
-940.68700E+00 -2.4124130E+00  2.5000000E+00  0.0000000E+00  0.0000000E+00     3
 0.0000000E+00  0.0000000E+00 -745.37510E+00  0.9153489E+00                   4
B1O                    O   1              G  0300.00   5000.00  1000.00     1
 0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14    2
 0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04    3
-0.01602843E-07 0.03890696E-11 0.02914764E+06 0.02963995E+02                   4
B2CO                   C   1O   1          G  0300.00   5000.00  1000.00     1
 0.03025078E+02 0.01442689E-01-0.05630828E-05 0.01018581E-08-0.06910952E-13    2
-0.01426835E+06 0.06108218E+02 0.03262452E+02 0.01511941E-01-0.03881755E-04    3
 0.05581944E-07-0.02474951E-10-0.01431054E+06 0.04848897E+02                   4
B3C                    C   1              G  0300.00   5000.00  1000.00     1
 0.02602087E+02-0.01787081E-02 0.09087041E-06-0.01149933E-09 0.03310844E-14    2
 0.08542154E+06 0.04195177E+02 0.02498585E+02 0.08085777E-03-0.02697697E-05    3
 0.03040729E-08-0.01106652E-11 0.08545878E+06 0.04753459E+02                   4
B4CH                   C   1H   1          G  0300.00   5000.00  1000.00     1
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13    2
 0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04    3
 0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331588E+02                   4
B5CH2       CH2t       C   1H   2          G  0300.00   5000.00  1000.00     1
 0.03636408E+02 0.01933057E-01-0.01687016E-05-0.01009899E-08 0.01808256E-12    2
 0.04534134E+06 0.02156561E+02 0.03762237E+02 0.01159819E-01 0.02489585E-05    3
 0.08800836E-08-0.07332435E-11 0.04536791E+06 0.01712578E+02                   4
B6CH2       CH2s       C   1H   2          G  0300.00   5000.00  1000.00     1
 0.03552889E+02 0.02066788E-01-0.01914116E-05-0.01104673E-08 0.02021350E-12    2
 0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699089E-02 0.01025369E-04    3
 0.02492551E-07-0.01981266E-10 0.04989368E+06 0.05753207E+00                   4
H2                     C   0H   2O   0     G  0300.00   5000.00  1000.00     1
 2.50170E+00    1.78083E-03   -7.80013E-07    1.48437E-10   -1.03401E-14      2
-6.86891E+02    1.25553E+00    3.43853E+00    1.44314E-04   -1.08191E-07      3
 2.16839E-10   -5.54307E-14   -1.03749E+03   -3.92682E+00                    4
H2O                    C   0H   2O   1     G  0300.00   5000.00  1000.00     1
 2.68039E+00    3.09623E-03   -9.31393E-07    1.34865E-10   -7.70007E-15      2
-2.99236E+04    6.77857E+00    3.97559E+00   -4.41834E-04    2.45596E-06      3
-1.24431E-09    2.26702E-13   -3.02810E+04    7.71523E-02                    4
O2                     C   0H   0O   2     G  0300.00   5000.00  1000.00     1
 3.19345E+00    1.56657E-03   -6.90657E-07    1.32082E-10   -9.23577E-15      2
-1.05228E+03    5.96618E+00    3.08809E+00    1.60342E-03   -5.34550E-07      3
 2.80793E-11    2.98899E-15   -9.93828E+02    6.61069E+00                    4
H2O2                   C   0H   2O   2     G  0300.00   5000.00  1000.00     1
 5.20269E+00    3.07820E-03   -8.47786E-07    1.14867E-10   -6.24436E-15      2
-1.81737E+04   -2.81106E+00    2.79724E+00    9.30806E-03   -3.27081E-06      3
-3.91853E-09    2.63341E-12   -1.75951E+04    9.47142E+00                    4
CH4                    C   1H   4O   0     G  0300.00   5000.00  1000.00     1
 1.61991E+00    1.03080E-02   -3.71228E-06    6.14185E-10   -3.86748E-14      2
-1.00748E+04    9.98982E+00    2.31954E+00    6.54738E-03   -7.48051E-07      3
 2.60912E-09   -1.95537E-12   -9.99764E+03    7.24965E+00                    4
HCHO                   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
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 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
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
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-.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
 -.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
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 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
 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
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
C5H10Y                  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
-7.71759E+03   -8.25186E+00    8.75607E-01    4.50825E-02   -1.19396E-05       3
-1.06759E-08    6.26846E-12   -6.00243E+03    2.31246E+01                       4
C7H14Y                  C   7H  14O   0     G  0300.00   5000.00  1000.00      1
 1.29823E+01    4.28561E-02   -1.52528E-05    2.50016E-09   -1.56279E-13       2
-1.66002E+04   -4.18674E+01   -1.26883E+00    7.55135E-02   -2.39281E-05       3
-2.06665E-08    1.32665E-11   -1.26789E+04    3.26228E+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
C8H16Y                  C   8H  16O   0     G  0300.00   5000.00  1000.00      1
 1.51596E+01    4.85708E-02   -1.71931E-05    2.80789E-09   -1.75087E-13       2
-2.18184E+04   -5.23975E+01   -4.41749E-01    8.36371E-02   -2.50589E-05       3
-2.38749E-08    1.48932E-11   -1.74712E+04    2.93667E+01                       4
C3H5OOHY                C   3H   6O   2     G  0300.00   5000.00  1000.00      1
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 2.00076E+01    2.61984E-03    1.39391E-06   -5.74781E-10    5.52590E-14       2
-2.13195E+04   -8.52119E+01    1.65546E+00    3.51832E-02   -1.33368E-05       3
 1.75133E-10   -6.62806E-14   -1.45020E+04    1.61426E+01                      4
C6H11OOHZ              C   6H  12O   2     G  0300.00   5000.00  1000.00      1
 3.67613E+01    2.71618E-03    3.72783E-06   -1.27488E-09    1.15968E-13       2
-3.58348E+04   -1.71185E+02    2.38174E+00    6.38206E-02   -2.37923E-05       3
-2.55871E-10    9.46987E-14   -2.30847E+04    1.86218E+01                      4
C4H7OOHY               C   4H   8O   2     G  0300.00   5000.00  1000.00      1
 2.52156E+01    3.17708E-03    2.06929E-06   -8.13080E-10    7.72326E-14       2
-2.58285E+04   -1.11261E+02    2.07864E+00    4.38798E-02   -1.54115E-05       3
-1.04949E-09    3.71163E-13   -1.72157E+04    1.66062E+01                      4
C5H9OOHZ               C   5H  10O   2     G  0300.00   5000.00  1000.00      1
 3.09964E+01    2.92194E-03    2.91806E-06   -1.04837E-09    9.69157E-14       2
-3.08327E+04   -1.41262E+02    2.13447E+00    5.45221E-02   -2.12332E-05       3
 9.90351E-10   -3.52845E-13   -2.01400E+04    1.80182E+01                      4
C7H13OOHY              C   7H  14O   2     G  0300.00   5000.00  1000.00      1
 4.45114E+01    4.47839E-04    4.65862E-06   -1.40115E-09    1.21728E-13       2
-4.40994E+04   -2.16851E+02    1.04392E+00    7.82134E-02   -3.13229E-05       3
 9.26809E-10   -3.26213E-13   -2.80132E+04    2.29732E+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
C7H15CHO               C   8H  16O   1     G  0300.00   5000.00  1000.00      1
 1.80131E+01    4.73870E-02   -1.64394E-05    2.64667E-09   -1.63385E-13       2
-4.70929E+04   -6.49286E+01   -3.28529E+00    1.01710E-01   -5.40806E-05       3
-5.81287E-10    7.64821E-12   -4.11645E+04    4.58157E+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
-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   -6.63310E+01    4.84381E+00    7.63010E-02   -3.17526E-05       3
-7.45549E-09    7.30401E-12   -4.63643E+04    1.68551E+01                      4
C7H14CHOOOH            C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 2.34007E+01    4.58018E-02   -1.53548E-05    2.41072E-09   -1.46115E-13       2
-5.82798E+04   -8.43852E+01   -1.22819E+00    1.10258E-01   -6.32868E-05       3
 2.95991E-09    7.38667E-12   -5.15453E+04    4.31889E+01                      4
C7H15COOOH             C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 2.16700E+01    4.81255E-02   -1.63396E-05    2.58515E-09   -1.57345E-13       2
-6.92224E+04   -7.78788E+01   -6.18935E+00    1.27782E-01   -8.98297E-05       3
 2.12451E-08    2.82856E-12   -6.19570E+04    6.46884E+01                      4
C2H5COOOH              C   3H   6O   3     G  0300.00   5000.00  1000.00      1
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 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
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
 1.60536E+01    2.91142E-02   -9.63156E-06    1.49697E-09   -9.00408E-14       2
-4.58349E+04   -4.87555E+01    4.08288E-01    7.03787E-02   -4.14097E-05       3
 3.48617E-09    4.06061E-12   -4.15566E+04    3.22419E+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
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
 1.35912E+01    2.58934E-02   -8.49175E-06    1.31368E-09   -7.88697E-14       2
-3.28210E+04   -3.92450E+01    1.38351E+00    5.78663E-02   -3.28684E-05       3
 2.62115E-09    3.20629E-12   -2.94582E+04    2.40410E+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   -3.87464E+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
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
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
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
-4.10939E+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
C8H17OOH                C   8H  18O   2     G  0300.00   5000.00  1000.00      1
 2.29499E+01    4.83522E-02   -1.61392E-05    2.52633E-09   -1.52821E-13       2
-4.79660E+04   -8.70196E+01   -5.35129E-02    1.03740E-01   -4.60601E-05       3
-1.20768E-08    1.19758E-11   -4.14579E+04    3.32905E+01                      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
C3H5OHY                 C   3H   6O   1     G  0300.00   5000.00  1000.00      1
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 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
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
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
C6H11OHY              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
C6H10YZ               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
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
 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
C7H13OHY              C   7H  14O   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
C7H12YZ               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
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
C10H18Y2              C  10H  18O   0     G  0300.00   5000.00  1000.00      1
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 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
C11H20Y2               C  11H  20O   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
C12H22Y2               C  12H  22O   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
C13H24Y2               C  13H  24O   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
C7H13CHOY              C   8H  14O   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
C8H15OHY               C   8H  16O   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
C9H18Y                 C   9H  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
C14H26Y2               C  14H  26O   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
C15H28Y2               C  15H  28O   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
C8H15OOHY              C   8H  16O   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
C8H15CHOY              C   9H  16O   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
C9H17OHY               C   9H  18O   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
C10H20Y                C  10H  20O   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
C16H30Y2               C  16H  30O   0     G  0300.00   5000.00  1000.00      1
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 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   -1.34619E+00   -9.24908E-01    2.64513E-02   -1.34725E-05       3
 3.74058E-10    1.40310E-12   -7.13279E+03    2.71327E+01                      4
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
-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   -5.02285E+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
-4.21611E+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
C8H16O#4               C   8H  16O   1     G  0300.00   5000.00  1000.00      1
 1.02102E+01    6.27816E-02   -2.42914E-05    4.22889E-09   -2.76095E-13       2
-3.15933E+04   -2.78903E+01   -8.66174E-03    6.75717E-02    3.00216E-05       3
-7.87501E-08    3.38285E-11   -2.79500E+04    2.98859E+01                      4
C8H16O#5               C   8H  16O   1     G  0300.00   5000.00  1000.00      1
 2.00102E+01    4.69426E-02   -1.66320E-05    2.71998E-09   -1.69879E-13       2
-4.81128E+04   -8.25320E+01    2.76191E+00    6.71252E-02    3.74334E-05       3
-9.57628E-08    4.13980E-11   -4.26705E+04    1.18353E+01                      4
C8H16O#6               C   8H  16O   1     G  0300.00   5000.00  1000.00      1
 1.97159E+01    4.69907E-02   -1.65932E-05    2.70705E-09   -1.68775E-13       2
-4.75591E+04   -8.16624E+01   -6.72175E-01    8.74665E-02   -1.20492E-05       3
-4.61334E-08    2.40604E-11   -4.15593E+04    2.66487E+01                      4
C8H16O#3               C   8H  16O   1     G  0300.00   5000.00  1000.00      1
 1.97048E+01    4.53654E-02   -1.55770E-05    2.48672E-09   -1.52445E-13       2
-3.77044E+04   -7.80974E+01    1.41542E+00    7.17630E-02    1.74103E-05       3
-6.89401E-08    3.02264E-11   -3.18286E+04    2.15642E+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
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 5.50836E+00    4.29493E-02   -1.73432E-05    3.11330E-09   -2.07830E-13       2
-2.32692E+04   -5.76833E+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
-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
 1.05037E+01    2.05791E-02   -7.22156E-06    1.17160E-09   -7.26883E-14       2
-3.19927E+04   -2.66891E+01   -1.10746E+00    4.97149E-02   -2.37319E-05       3
-6.80564E-09    6.88541E-12   -2.88433E+04    3.35568E+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   -9.12456E+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
 2.08715E+01    3.99415E-02   -1.32621E-05    2.06845E-09   -1.24819E-13       2
-3.98816E+04   -7.08402E+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
C8H15O#4OOH            C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 1.77697E+01    5.74585E-02   -2.12173E-05    3.57068E-09   -2.27432E-13       2
-5.09027E+04   -6.31533E+01   -1.01947E+01    1.48472E-01   -1.28609E-04       3
 5.49960E-08   -7.42194E-12   -4.40656E+04    7.73568E+01                      4
C8H15O#5OOH            C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 2.55347E+01    4.50964E-02   -1.53770E-05    2.44210E-09   -1.49137E-13       2
-5.93542E+04   -1.03152E+02    4.85817E+00    7.53657E-02    2.90767E-05       3
-9.32068E-08    4.15368E-11   -5.30551E+04    8.64156E+00                      4
C8H15O#6OOH            C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 2.53121E+01    4.40782E-02   -1.47357E-05    2.30823E-09   -1.39641E-13       2
-6.38300E+04   -1.05338E+02    2.46254E+00    7.79087E-02    3.47152E-05       3
-1.04730E-07    4.65719E-11   -5.69620E+04    1.79469E+01                      4
C8H15O#3OOH            C   8H  16O   3     G  0300.00   5000.00  1000.00      1
 2.59544E+01    4.17841E-02   -1.35604E-05    2.08258E-09   -1.24419E-13       2
-5.43719E+04   -1.05709E+02   -1.61298E+00    1.03891E-01   -3.24638E-05       3
-3.54301E-08    2.17839E-11   -4.65602E+04    3.90917E+01                      4
C5H9O#3OOH             C   5H  10O   3     G  0300.00   5000.00  1000.00      1
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 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
-4.99409E+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
C6H10#ZOOY              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
C4H#3OH10COYCOOH        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
C8H14#ZYZ               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
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
C9H16#ZYZ               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
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
 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
C7H13O#4COOOH           C   8H  14O   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
C7H13O#5COOOH           C   8H  14O   4     G  0300.00   5000.00  1000.00      1
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 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#6COOOH            C   8H  14O   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
R21C7H15                 C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.26181E+01    4.32427E-02   -1.41265E-05    2.17861E-09   -1.30476E-13       2
-5.28170E+03   -3.33717E+01   -7.69115E-01    8.48580E-02   -5.80163E-05       3
 1.92553E-08   -1.52775E-12   -2.06189E+03    3.40905E+01                      4
R22C7H15                 C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.26181E+01    4.32427E-02   -1.41265E-05    2.17861E-09   -1.30476E-13       2
-5.28170E+03   -3.26786E+01   -7.69115E-01    8.48580E-02   -5.80163E-05       3
 1.92553E-08   -1.52775E-12   -2.06189E+03    3.47836E+01                      4
R23C7H15                 C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.24886E+01    4.35229E-02   -1.42351E-05    2.19307E-09   -1.31016E-13       2
-5.28122E+03   -3.20716E+01    4.20035E-01    7.64520E-02   -3.89751E-05       3
 1.58108E-09    4.37549E-12   -2.17894E+03    2.98130E+01                      4
R24C7H15                 C   7H  15O   0     G  0300.00   5000.00  1000.00      1
 1.29086E+01    4.33460E-02   -1.42538E-05    2.21035E-09   -1.32981E-13       2
-4.88191E+03   -3.45892E+01   -4.37596E-01    8.15899E-02   -4.75138E-05       3
 7.98694E-09    2.46307E-12   -1.53436E+03    3.34147E+01                      4
R25C8H17                 C   8H  17O   0     G  0300.00   5000.00  1000.00      1
 1.65781E+01    4.79568E-02   -1.58330E-05    2.45887E-09   -1.47904E-13       2
-1.13887E+04   -5.77977E+01   -2.45792E+00    1.00416E-01   -5.52412E-05       3
 8.18171E-10    7.48841E-12   -6.56322E+03    3.95814E+01                      4
R26C8H17                 C   8H  17O   0     G  0300.00   5000.00  1000.00      1
 1.62241E+01    4.79657E-02   -1.57712E-05    2.44271E-09   -1.46688E-13       2
-1.16622E+04   -5.66316E+01   -2.80712E+00    1.03796E-01   -6.59900E-05       3
 1.23120E-08    3.42374E-12   -6.98806E+03    3.99281E+01                      4
R27C8H17                 C   8H  17O   0     G  0300.00   5000.00  1000.00      1
 1.54473E+01    4.88291E-02   -1.61009E-05    2.49663E-09   -1.49924E-13       2
-1.33793E+04   -5.27801E+01   -8.35087E-01    9.07781E-02   -3.96894E-05       3
-1.04780E-08    1.07794E-11   -9.15081E+03    3.11321E+01                      4
R28C8H17                 C   8H  17O   0     G  0300.00   5000.00  1000.00      1
 1.65979E+01    4.79226E-02   -1.58133E-05    2.45430E-09   -1.47533E-13       2
-1.27050E+04   -5.83133E+01   -2.57455E+00    1.01220E-01   -5.71585E-05       3
 2.71860E-09    6.82038E-12   -7.85904E+03    3.96706E+01                      4
R29C3H7OO                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
-1.05996E+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
R30C4H9OO                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
R31C7H15OO               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
R32C7H15OO               C   7H  15O   2     G  0300.00   5000.00  1000.00      1
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 2.22245E+01    3.63956E-02   -1.09858E-05    1.60073E-09   -9.21346E-14       2
-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
R33C7H15OO              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
R34C7H15OO              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
R35C5H11                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
R36C8H17OO              C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.61790E+01    4.02621E-02   -1.21840E-05    1.77416E-09   -1.01822E-13       2
-3.13356E+04   -1.06205E+02   -1.33130E+00    1.07392E-01   -5.66082E-05       3
-2.14473E-09    8.62014E-12   -2.33467E+04    3.80377E+01                      4
R37C4H9                 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
 3.95673E+03   -1.81633E+01   -1.27500E+00    5.39217E-02   -4.19539E-05       3
 1.75003E-08   -2.65793E-12    6.31568E+03    3.04740E+01                      4
R38C8H17OO              C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.62593E+01    4.03680E-02   -1.22510E-05    1.78708E-09   -1.02664E-13       2
-3.33126E+04   -1.07806E+02    2.94226E+00    7.88952E-02    1.36336E-05       3
-7.23591E-08    3.30247E-11   -2.59763E+04    1.82269E+01                      4
R39C8H17OO              C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.64603E+01    4.02247E-02   -1.22224E-05    1.78681E-09   -1.02934E-13       2
-3.54045E+04   -1.10119E+02    2.22274E+00    8.62136E-02   -5.10677E-06       3
-5.37951E-08    2.66740E-11   -2.79932E+04    1.95946E+01                      4
R40C4H9                 C   4H   9O   0     G  0300.00   5000.00  1000.00      1
 5.08707E+00    2.68389E-02   -8.54487E-06    1.29347E-09   -7.64449E-14       2
 2.24900E+03   -2.82482E-01    9.74119E-01    2.72246E-02    1.46405E-05       3
-3.00628E-08    1.18088E-11    3.90265E+03    2.36312E+01                      4
R41C8H17OO              C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.61399E+01    4.03317E-02   -1.22250E-05    1.78388E-09   -1.02623E-13       2
-3.13197E+04   -1.06392E+02   -1.25465E+00    1.06868E-01   -5.53692E-05       3
-3.36219E-09    9.04460E-12   -2.33547E+04    3.73075E+01                      4
R42C5H11                C   5H  11O   0     G  0300.00   5000.00  1000.00      1
 1.05898E+01    2.95322E-02   -9.40443E-06    1.42399E-09   -8.41867E-14       2
-1.10763E+03   -3.07391E+01   -9.36358E-01    5.79230E-02   -2.40470E-05       3
-8.15421E-09    7.27552E-12    2.02656E+03    2.91639E+01                      4
R43C3H6OOH              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
-4.14964E+03   -4.01390E+01    1.79245E+00    4.81646E-02   -4.60604E-05       3
 2.62519E-08   -6.46414E-12   -7.91460E+02    2.16932E+01                      4
R44C3H6OOH              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
-3.81449E+03   -4.35349E+01    8.95897E-01    5.35669E-02   -5.52210E-05       3
 3.32666E-08   -8.58837E-12   -1.42826E+02    2.54605E+01                      4
R45C4H8OOH              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
-7.77919E+03   -5.12759E+01    7.20942E-01    6.62556E-02   -6.70288E-05       3
 4.02798E-08   -1.03878E-11   -3.61597E+03    2.79664E+01                      4
R46C4H8OOH              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
-7.74929E+03   -5.03054E+01    1.73881E+00    5.90464E-02   -5.08822E-05       3
 2.55120E-08   -5.51809E-12   -3.71481E+03    2.37199E+01                      4
R47C4H8OOH              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
-7.41103E+03   -5.36611E+01    1.06688E+00    6.28975E-02   -5.63346E-05       3
 2.88426E-08   -6.34414E-12   -3.09031E+03    2.65350E+01                      4
R48C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
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 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
R49C7H14OOH             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
R50C7H14OOH             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   -1.44763E+04    1.44503E+01                      4
R51C7H14OOH             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
R52C7H14OOH             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   -1.44763E+04    1.44503E+01                      4
R53C7H14OOH             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
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
 2.26526E+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
R56C7H14OOH             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   -1.44763E+04    1.44503E+01                      4
R57C7H14OOH             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
R58C7H14OOH             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   -1.50033E+04    1.58281E+01                      4
R59C7H14OOH             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
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
 2.26526E+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
R62C7H14OOH             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
-1.84883E+04   -8.02760E+01    9.03075E-01    9.65757E-02   -7.60396E-05       3
 3.27376E-08   -5.70540E-12   -1.24235E+04    3.25784E+01                      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
-1.84883E+04   -8.02760E+01    9.03075E-01    9.65757E-02   -7.60396E-05       3
 3.27376E-08   -5.70540E-12   -1.24235E+04    3.25784E+01                      4
R64C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
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 2.28035E+01    3.42678E-02   -9.92812E-06    1.39923E-09   -7.84001E-14       2
-1.84978E+04   -8.04125E+01    7.60335E-01    9.75635E-02   -7.84072E-05       3
 3.50961E-08   -6.53860E-12   -1.24082E+04    3.31832E+01                      4
R65C7H14OOH             C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.28035E+01    3.42678E-02   -9.92812E-06    1.39923E-09   -7.84001E-14       2
-1.84978E+04   -8.04125E+01    7.60335E-01    9.75635E-02   -7.84072E-05       3
 3.50961E-08   -6.53860E-12   -1.24082E+04    3.31832E+01                      4
R66C5H11OO              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
-1.77326E+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
R67C5H11                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
 1.18006E+03   -2.20876E+01    1.26900E-01    5.75816E-02   -3.65250E-05       3
 1.05183E-08   -2.59295E-13    3.69897E+03    2.74231E+01                      4
R68C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.71167E+01    3.83496E-02   -1.13164E-05    1.61674E-09   -9.14841E-14       2
-2.51183E+04   -1.06737E+02   -8.29629E-01    1.12248E-01   -7.32809E-05       3
 1.43051E-08    3.23918E-12   -1.73043E+04    3.83316E+01                      4
R69C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.67218E+01    3.84424E-02   -1.13097E-05    1.61354E-09   -9.12862E-14       2
-2.53763E+04   -1.04940E+02   -1.75964E+00    1.19647E-01   -9.36577E-05       3
 3.53840E-08   -4.20929E-12   -1.76667E+04    4.15448E+01                      4
R70C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.59445E+01    3.92930E-02   -1.16250E-05    1.66430E-09   -9.43345E-14       2
-2.70908E+04   -1.01080E+02    4.79837E-01    1.04772E-01   -6.28975E-05       3
 8.14476E-09    4.71935E-12   -1.98578E+04    3.16164E+01                      4
R71C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.70891E+01    3.83983E-02   -1.13449E-05    1.62350E-09   -9.20432E-14       2
-2.64151E+04   -1.06582E+02   -1.04617E+00    1.13727E-01   -7.67841E-05       3
 1.77560E-08    2.03180E-12   -1.85892E+04    3.92518E+01                      4
R72C4H9OO               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   -5.58325E+01    5.76065E-02    5.93770E-02   -3.93844E-05       3
 1.02650E-08    1.27553E-13   -1.05891E+04    2.80846E+01                      4
R73C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.59673E+01    3.94986E-02   -1.17491E-05    1.69063E-09   -9.62759E-14       2
-2.86414E+04   -1.02359E+02    4.63771E+00    7.70682E-02    5.46587E-06       3
-6.02176E-08    2.84759E-11   -2.20723E+04    1.22966E+01                      4
R74C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.71659E+01    3.85094E-02   -1.14144E-05    1.63712E-09   -9.29552E-14       2
-2.79876E+04   -1.08162E+02    3.02995E+00    8.66052E-02   -9.85415E-06       3
-4.91436E-08    2.52607E-11   -2.07952E+04    2.02761E+01                      4
R75C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.72221E+01    3.84095E-02   -1.13557E-05    1.62319E-09   -9.18059E-14       2
-2.67019E+04   -1.08070E+02    3.09390E+00    8.61752E-02   -8.85206E-06       3
-5.01171E-08    2.55975E-11   -1.94938E+04    2.04087E+01                      4
R76C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.74204E+01    3.82718E-02   -1.13308E-05    1.62381E-09   -9.21496E-14       2
-2.87930E+04   -1.10775E+02    2.41746E+00    9.31832E-02   -2.68207E-05       3
-3.23464E-08    1.95342E-11   -2.15152E+04    2.11901E+01                      4
R77C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.70696E+01    3.82864E-02   -1.12782E-05    1.60971E-09   -9.10521E-14       2
-2.90703E+04   -1.09228E+02    2.36501E+00    9.45180E-02   -3.26849E-05       3
-2.57031E-08    1.71787E-11   -2.19718E+04    2.06837E+01                      4
R78C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.73712E+01    3.83586E-02   -1.13815E-05    1.63577E-09   -9.31298E-14       2
-2.87732E+04   -1.10095E+02    2.50075E+00    9.26035E-02   -2.54239E-05       3
-3.37434E-08    2.00293E-11   -2.15241E+04    2.12430E+01                      4
R79C4H9OO               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
-1.86293E+04   -6.02768E+01    3.56632E+00    3.85065E-02    1.13947E-05       3
-4.06792E-08    1.79361E-11   -1.44256E+04    9.83378E+00                      4
R80C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
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 2.61728E+01    3.88487E-02   -1.14258E-05    1.62829E-09   -9.19689E-14       2
-2.71335E+04   -1.02651E+02   -5.46283E-01    1.12047E-01   -7.92181E-05       3
 2.30991E-08   -2.19500E-13   -1.97582E+04    3.54912E+01                      4
R81C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.70321E+01    3.85012E-02   -1.14060E-05    1.63808E-09   -9.32479E-14       2
-2.63925E+04   -1.07363E+02   -1.07287E+00    1.13935E-01   -7.73363E-05       3
 1.83531E-08    1.80677E-12   -1.85867E+04    3.82631E+01                      4
R82C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.67218E+01    3.84424E-02   -1.13097E-05    1.61354E-09   -9.12862E-14       2
-2.53763E+04   -1.05346E+02   -1.75964E+00    1.19647E-01   -9.36577E-05       3
 3.53840E-08   -4.20929E-12   -1.76667E+04    4.11394E+01                      4
R83C8H16OOH             C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.71297E+01    3.83290E-02   -1.13056E-05    1.61448E-09   -9.13187E-14       2
-2.51241E+04   -1.06811E+02   -7.72081E-01    1.11838E-01   -7.22727E-05       3
 1.32787E-08    3.60831E-12   -1.73103E+04    3.80894E+01                      4
R84C5H11OO              C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 1.95980E+01    2.33518E-02   -6.58768E-06    9.10840E-10   -5.03664E-14       2
-2.07345E+04   -7.64749E+01   -7.39096E-01    7.39282E-02   -4.36285E-05       3
 3.37106E-09    4.29214E-12   -1.48223E+04    3.00467E+01                      4
R85C3H6OOOOH            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
-2.38741E+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
R86C3H6OOOOH            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
-2.15524E+04   -6.02423E+01    2.64693E+00    5.58589E-02   -4.42549E-05       3
 1.66943E-08   -2.10627E-12   -1.70895E+04    2.13235E+01                      4
R87C4H8OOOOH            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
-2.74730E+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
R88C4H8OOOOH            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   -2.21320E+04    2.45830E+01                      4
R89C4H8OOOOH            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
-2.51679E+04   -7.13117E+01    2.78837E+00    6.54017E-02   -4.58976E-05       3
 1.28194E-08   -6.40537E-14   -2.00339E+04    2.18256E+01                      4
R90C4H8OOH              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
-1.09469E+04   -5.11833E+01    8.38706E-01    6.54180E-02   -6.52570E-05       3
 3.87153E-08   -9.88741E-12   -6.79692E+03    2.74756E+01                      4
R91C7H14OOOOH           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
-4.05381E+04   -1.08665E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29550E+04    3.37796E+01                      4
R92C7H14OOOOH           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   -1.09160E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.52957E+01                      4
R93C7H14OOOOH           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
-3.78998E+04   -1.00773E+02    6.78748E+00    7.03730E-02    7.81416E-06       3
-5.74652E-08    2.63872E-11   -3.14219E+04    1.03497E+01                      4
R94C7H14OOH             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
-2.43716E+04   -7.99258E+01    4.62134E+00    7.29023E-02   -1.97553E-05       3
-2.29980E-08    1.36357E-11   -1.90808E+04    1.49446E+01                      4
R95C5H10OOH             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
-1.43464E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -1.00532E+04    9.81073E+00                      4
R96C7H14OOOOH           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.86583E+01    3.40280E-02   -9.79680E-06    1.37670E-09   -7.71072E-14       2
-4.05730E+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
R97C7H14OOOOH           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
-3.79002E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57566E+00                      4
R98C5H10OOH             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   -9.72302E+03    2.93985E+01                      4
R99C7H14OOOOH           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    9.60741E-01    1.10162E-01   -8.01649E-05       3
 2.30258E-08    1.82638E-13   -3.29512E+04    3.39337E+01                      4
R100C7H14OOOOH          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
-4.05381E+04   -1.08665E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29550E+04    3.37797E+01                      4
R101C3H6OOH             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
-7.34154E+03   -4.09293E+01    6.87659E-01    5.59501E-02   -6.38155E-05       3
 4.28124E-08   -1.20157E-11   -3.85159E+03    2.63165E+01                      4
R102C7H14OOOOH          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   -1.09160E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.52957E+01                      4
R103C7H14OOH            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
-2.43716E+04   -7.92327E+01    4.62134E+00    7.29023E-02   -1.97553E-05       3
-2.29980E-08    1.36357E-11   -1.90808E+04    1.56377E+01                      4
R104C4H8OOH             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
-1.11436E+04   -5.77841E+01    2.10196E-01    6.91274E-02   -6.67008E-05       3
 3.56004E-08   -7.86517E-12   -6.57050E+03    2.96529E+01                      4
R105C7H14OOOOH          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   -3.14186E+04    1.04788E+01                      4
R106C5H10OOH            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
-1.29374E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -8.64421E+03    9.81073E+00                      4
R107C7H14OOOOH          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
-3.79002E+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
R108C7H14OOH            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   -1.44763E+04    1.44503E+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
-4.05731E+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
R110C7H14OOOOH          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    9.60741E-01    1.10162E-01   -8.01649E-05       3
 2.30258E-08    1.82638E-13   -3.29512E+04    3.46268E+01                      4
R111C7H14OOOOH          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
-4.05381E+04   -1.07972E+02    9.97524E-01    1.09898E-01   -7.95079E-05       3
 2.23498E-08    4.28218E-13   -3.29550E+04    3.44727E+01                      4
R112C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
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 2.22173E+01    3.50130E-02   -1.02532E-05    1.46132E-09   -8.28015E-14       2
-2.42924E+04   -7.75536E+01    5.82425E+00    6.44188E-02   -5.68825E-07       3
-4.07814E-08    1.95668E-11   -1.91995E+04    1.06062E+01                      4
R113C3H6OOH             C   3H   7O   2     G  0300.00   5000.00  1000.00      1
 1.50221E+01    1.15175E-02   -2.68435E-06    3.19846E-10   -1.57998E-14       2
-7.52668E+03   -4.73815E+01    3.97669E-01    5.73200E-02   -5.96743E-05       3
 3.41718E-08   -8.05761E-12   -3.66146E+03    2.70592E+01                      4
R114C7H14OOOOH          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   -1.08467E+02    6.39545E-01    1.12390E-01   -8.55107E-05       3
 2.83536E-08   -1.69946E-12   -3.29168E+04    3.59887E+01                      4
R115C4H8OOH             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
-9.71422E+03   -5.75014E+01    2.65192E-01    6.87533E-02   -6.58213E-05       3
 3.47408E-08   -7.56690E-12   -5.16746E+03    2.94190E+01                      4
R116C7H14OOOOH          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
-3.79002E+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
R117C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.25857E+01    3.46949E-02   -1.01179E-05    1.43329E-09   -8.06282E-14       2
-1.84600E+04   -7.93079E+01    1.98283E+00    8.89205E-02   -5.87839E-05       3
 1.68305E-08   -4.22925E-13   -1.25287E+04    2.80722E+01                      4
R118C7H14OOH            C   7H  15O   2     G  0300.00   5000.00  1000.00      1
 2.31841E+01    3.42012E-02   -9.95055E-06    1.40639E-09   -7.89451E-14       2
-1.81323E+04   -8.28191E+01    1.02078E+00    9.47897E-02   -6.90957E-05       3
 2.50204E-08   -2.97103E-12   -1.18733E+04    3.21151E+01                      4
R119C7H14OOOOH          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
-3.79002E+04   -1.01467E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57582E+00                      4
R120C7H14OOOOH          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
-3.79002E+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
R121C7H14OOH            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
-2.16373E+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
R122C7H14OOOOH          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
-3.79002E+04   -1.01466E+02    7.04271E+00    6.86049E-02    1.20546E-05       3
-6.16903E-08    2.78797E-11   -3.14492E+04    8.57644E+00                      4
R123C5H10OOH            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
-1.13670E+04   -6.12307E+01    6.25544E-01    7.74532E-02   -7.26708E-05       3
 4.04136E-08   -9.76785E-12   -6.53523E+03    3.01646E+01                      4
R124C5H10OOH            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
-1.13670E+04   -6.12307E+01    6.25544E-01    7.74532E-02   -7.26708E-05       3
 4.04136E-08   -9.76785E-12   -6.53523E+03    3.01646E+01                      4
R125C5H10OOH            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
-1.13136E+04   -5.99212E+01    1.86607E+00    6.86882E-02   -5.27615E-05       3
 2.18688E-08   -3.55540E-12   -6.65774E+03    2.49768E+01                      4
R126C5H10OOH            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
-1.09850E+04   -6.34124E+01    1.10965E+00    7.31303E-02   -5.96440E-05       3
 2.66359E-08   -4.89249E-12   -6.02427E+03    2.81490E+01                      4
R127C5H11OO             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   -1.52017E+04    9.73754E+00                      4
R128C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
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 3.12917E+01    3.92720E-02   -1.14955E-05    1.63072E-09   -9.17048E-14       2
-4.28382E+04   -1.25286E+02    7.66149E-01    1.15621E-01   -6.49312E-05       3
 3.70399E-10    8.77610E-12   -3.41337E+04    3.41493E+01                      4
R129C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.11894E+01    3.96996E-02   -1.17505E-05    1.68813E-09   -9.62085E-14       2
-4.47408E+04   -1.25460E+02    4.88546E+00    8.81941E-02    2.74357E-06       3
-6.72842E-08    3.22758E-11   -3.67468E+04    1.53975E+01                      4
R130C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.15938E+01    3.91965E-02   -1.15112E-05    1.63798E-09   -9.23760E-14       2
-4.65120E+04   -1.28907E+02    4.02095E+00    9.65218E-02   -1.84284E-05       3
-4.62891E-08    2.50642E-11   -3.83457E+04    1.73789E+01                      4
R131C8H16OOH            C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.67471E+01    3.83699E-02   -1.12601E-05    1.60100E-09   -9.02206E-14       2
-2.85622E+04   -1.05091E+02   -1.22439E+00    1.15895E-01   -8.48449E-05       3
 2.67557E-08   -1.19863E-12   -2.08920E+04    3.92886E+01                      4
R132C4H8OOH             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
-1.06466E+04   -5.01469E+01    2.02910E+00    5.56390E-02   -4.29719E-05       3
 1.78446E-08   -2.81018E-12   -6.71503E+03    2.09829E+01                      4
R133C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12565E+01    3.93349E-02   -1.15327E-05    1.63952E-09   -9.24302E-14       2
-4.28241E+04   -1.24395E+02    7.81336E-01    1.15518E-01   -6.46881E-05       3
 1.31810E-10    8.85934E-12   -3.41354E+04    3.47792E+01                      4
R134C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 2.04192E+01    2.16772E-02   -5.87404E-06    7.88659E-10   -4.27257E-14       2
-1.40742E+04   -7.59696E+01   -3.30333E-01    7.94170E-02   -6.17933E-05       3
 2.12839E-08   -1.59837E-12   -8.36750E+03    3.11402E+01                      4
R135C4H8OOH             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
-9.97841E+03   -5.57410E+01    3.67056E-01    6.55525E-02   -5.91959E-05       3
 2.98204E-08   -6.34422E-12   -5.43204E+03    2.91923E+01                      4
R136C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.28659E+01    3.78803E-02   -1.10374E-05    1.56334E-09   -8.79780E-14       2
-4.91701E+04   -1.37582E+02   -1.74872E+00    1.35975E-01   -1.05796E-04       3
 3.38358E-08   -1.10271E-12   -3.98818E+04    4.03080E+01                      4
R137C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12532E+01    3.95881E-02   -1.16859E-05    1.67299E-09   -9.49729E-14       2
-4.43644E+04   -1.25529E+02    4.96543E+00    8.76262E-02    4.13797E-06       3
-6.87029E-08    3.27861E-11   -3.63526E+04    1.53492E+01                      4
R138C5H10OOH            C   5H  11O   2     G  0300.00   5000.00  1000.00      1
 2.00668E+01    2.16695E-02   -5.80220E-06    7.68707E-10   -4.10596E-14       2
-1.75254E+04   -7.48261E+01   -7.48944E-01    8.32468E-02   -7.38337E-05       3
 3.42442E-08   -6.22665E-12   -1.19529E+04    3.17904E+01                      4
R139C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12532E+01    3.95881E-02   -1.16859E-05    1.67299E-09   -9.49729E-14       2
-4.43642E+04   -1.25123E+02    4.80216E+00    8.87618E-02    1.40404E-06       3
-6.59698E-08    3.18179E-11   -3.63352E+04    1.64446E+01                      4
R140C4H8OOH             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
-1.20736E+04   -5.35148E+01    1.10111E-01    6.82705E-02   -6.85864E-05       3
 4.01522E-08   -1.00468E-11   -7.72653E+03    2.95619E+01                      4
R141C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.14756E+01    3.94054E-02   -1.16333E-05    1.66680E-09   -9.47401E-14       2
-4.64648E+04   -1.28655E+02    4.36184E+00    9.41416E-02   -1.26786E-05       3
-5.20523E-08    2.71099E-11   -3.83819E+04    1.55314E+01                      4
R142C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.28869E+01    3.78425E-02   -1.10152E-05    1.55810E-09   -8.75490E-14       2
-4.91787E+04   -1.37007E+02   -1.55520E+00    1.34637E-01   -1.02593E-04       3
 3.06513E-08    1.95323E-14   -3.99025E+04    4.01804E+01                      4
R143C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.15573E+01    3.92625E-02   -1.15507E-05    1.64750E-09   -9.31704E-14       2
-4.64982E+04   -1.28707E+02    4.36801E+00    9.41064E-02   -1.26103E-05       3
-5.21075E-08    2.71257E-11   -3.83827E+04    1.59099E+01                      4
R144C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
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 1.72144E+01    1.70748E-02   -4.41399E-06    5.70281E-10   -2.99530E-14       2
-1.19539E+04   -5.95444E+01    3.78554E+00    4.53128E-02   -9.94330E-06       3
-1.95904E-08    1.09188E-11   -7.95048E+03    1.17284E+01                      4
R145C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.15190E+01    3.93283E-02   -1.15881E-05    1.65611E-09   -9.38616E-14       2
-4.68847E+04   -1.28897E+02    4.22586E+00    9.50894E-02   -1.49647E-05       3
-4.97637E-08    2.62983E-11   -3.87700E+04    1.61065E+01                      4
R146C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.11671E+01    3.94944E-02   -1.16265E-05    1.66172E-09   -9.42529E-14       2
-4.27885E+04   -1.25690E+02    8.34137E-01    1.15149E-01   -6.37947E-05       3
-7.67456E-10    9.18033E-12   -3.41410E+04    3.27633E+01                      4
R147C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.13158E+01    3.94752E-02   -1.16189E-05    1.65704E-09   -9.36561E-14       2
-4.47914E+04   -1.26570E+02    4.74924E+00    8.91251E-02    5.40221E-07       3
-6.51147E-08    3.15172E-11   -3.67320E+04    1.55707E+01                      4
R148C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12917E+01    3.92720E-02   -1.14955E-05    1.63072E-09   -9.17048E-14       2
-4.28383E+04   -1.24592E+02    8.66411E-01    1.14920E-01   -6.32314E-05       3
-1.33985E-09    9.38567E-12   -3.41444E+04    3.44192E+01                      4
R149C8H16OOH            C   8H  17O   2     G  0300.00   5000.00  1000.00      1
 2.66942E+01    3.84634E-02   -1.13147E-05    1.61385E-09   -9.12723E-14       2
-2.85405E+04   -1.05200E+02   -1.42456E+00    1.17296E-01   -8.82376E-05       3
 3.01666E-08   -2.41279E-12   -2.08708E+04    3.97292E+01                      4
R150C3H5O4H2            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   -6.43221E+01    2.36525E+00    6.64702E-02   -7.02729E-05       3
 3.90355E-08   -8.76023E-12   -1.40325E+04    2.30341E+01                      4
R151C3H5O4H2            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
-2.05557E+04   -6.17800E+01    2.21088E+00    6.84598E-02   -7.78745E-05       3
 4.75472E-08   -1.18084E-11   -1.63377E+04    2.36648E+01                      4
R152C3H6OOOOH           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   -1.92072E+04    2.19180E+01                      4
R153C3H5O4H2            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
-1.51136E+04   -5.90838E+01    2.77259E+00    6.42763E-02   -7.20994E-05       3
 4.50478E-08   -1.16929E-11   -1.10665E+04    2.10972E+01                      4
R154C3H5O4H2            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
-1.82714E+04   -5.81637E+01    2.77472E+00    6.42366E-02   -7.22327E-05       3
 4.53731E-08   -1.18572E-11   -1.42350E+04    2.17897E+01                      4
R155C4H7O4H2            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
-2.42228E+04   -7.29239E+01    2.20815E+00    7.89997E-02   -8.18940E-05       3
 4.60137E-08   -1.05816E-11   -1.92667E+04    2.54712E+01                      4
R156C4H8OOOOH           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
-2.74730E+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
R157C4H7O4H2            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
-2.10330E+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
R158C4H7O4H2            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
-2.06768E+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
R159C4H7O4H2            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   -1.69746E+04    2.43150E+01                      4
R160C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
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 2.16246E+01    1.67315E-02   -4.09709E-06    5.12477E-10   -2.65372E-14       2
-2.10348E+04   -7.27301E+01    2.23817E+00    7.88288E-02   -8.12855E-05       3
 4.52443E-08   -1.02699E-11   -1.61018E+04    2.53339E+01                      4
R161C4H7O4H2           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
-2.42179E+04   -7.28556E+01    2.18145E+00    7.91801E-02   -8.23160E-05       3
 4.64249E-08   -1.07241E-11   -1.92638E+04    2.55849E+01                      4
R162C4H8OOOOH          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
-2.75093E+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
R163C4H7O4H2           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
-1.87548E+04   -6.91822E+01    2.71540E+00    7.51980E-02   -7.70546E-05       3
 4.44777E-08   -1.08192E-11   -1.39897E+04    2.38270E+01                      4
R164C4H7O4H2           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
-2.19216E+04   -6.90817E+01    2.69095E+00    7.53338E-02   -7.75900E-05       3
 4.51878E-08   -1.11150E-11   -1.71552E+04    2.39403E+01                      4
R165C4H8OOOOH          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
-3.01394E+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
R166C7H13O4H2          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
-3.41691E+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
R167C7H13O4H2          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
-3.38256E+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
R168C7H13O4H2          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
-3.81143E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09649E+04    3.65169E+01                      4
R169C7H13O4H2          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
-3.42055E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69003E+04    3.62018E+01                      4
R170C7H13O4H2          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
-3.41691E+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
R171C7H13O4H2          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
-3.38256E+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
R172C7H13O4H2          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
-3.52346E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78005E+04    3.40991E+01                      4
R173C7H13O4H2          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   -2.69003E+04    3.62018E+01                      4
R174C7H13O4H2          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
-3.81143E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09649E+04    3.65169E+01                      4
R175C7H13O4H2          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
-3.42055E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69003E+04    3.62018E+01                      4
R176C7H13O4H2          C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.89610E+01    3.26925E-02   -9.15371E-06    1.25870E-09   -6.93334E-14       2
-3.41691E+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
R177C7H13O4H2           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   -2.54055E+04    1.05551E+01                      4
R178C7H13O4H2           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   -2.54055E+04    1.05551E+01                      4
R179C7H13O4H2           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
-3.54058E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94436E+04    1.19254E+01                      4
R180C7H13O4H2           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
-3.15215E+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
R181C7H14OOOOH          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
R182C5H10OOOOH          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
-3.07599E+04   -8.21560E+01    6.87268E+00    4.87349E-02    1.72258E-05       3
-5.58217E-08    2.44602E-11   -2.55724E+04    5.70995E+00                      4
R183C5H10OOH            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
-1.33136E+04   -6.07627E+01    6.00935E+00    4.10908E-02    1.53302E-05       3
-4.62069E-08    2.00942E-11   -9.27332E+03    6.81659E+00                      4
R184C5H10OOH            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
-1.29374E+04   -6.35904E+01    5.29541E+00    4.52254E-02    9.21607E-06       3
-4.22329E-08    1.90458E-11   -8.64421E+03    9.81073E+00                      4
R185C7H13O4H2           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
-3.52346E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78005E+04    3.40991E+01                      4
R186C7H13O4H2           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
-3.80909E+04   -1.05890E+02    3.87168E-01    1.24423E-01   -1.24462E-04       3
 6.83835E-08   -1.53706E-11   -3.09408E+04    3.74722E+01                      4
R187C7H13O4H2           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
-3.42055E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69003E+04    3.62018E+01                      4
R188C7H13O4H2           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
-3.42055E+04   -1.07749E+02    8.24526E-01    1.20404E-01   -1.12405E-04       3
 5.57766E-08   -1.09626E-11   -2.69003E+04    3.62018E+01                      4
R189C7H13O4H2           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
-3.41691E+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
R190C7H13O4H2           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   -2.54055E+04    1.05551E+01                      4
R191C7H13O4H2           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
-3.54058E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94436E+04    1.19254E+01                      4
R192C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.78567E+01    3.36466E-02   -9.46616E-06    1.30526E-09   -7.19862E-14       2
-3.15215E+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
R193C7H13O4H2           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
-3.15215E+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
R194C5H10OOOOH          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
-3.37535E+04   -8.23344E+01    3.74508E+00    5.87006E-02    3.83215E-06       3
-4.84538E-08    2.30184E-11   -2.79726E+04    1.98441E+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
-3.81143E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09649E+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
-3.41691E+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
R197C7H13O4H2           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
-3.38256E+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
R198C7H13O4H2           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   -2.69003E+04    3.55087E+01                      4
R199C7H13O4H2           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
-3.81143E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09649E+04    3.65169E+01                      4
R200C3H6OOOOH           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
-2.66996E+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
R201C7H13O4H2           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
-3.52346E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78005E+04    3.40991E+01                      4
R202C7H13O4H2           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   -2.69003E+04    3.62018E+01                      4
R203C7H13O4H2           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   -2.69003E+04    3.62018E+01                      4
R204C7H13O4H2           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
-3.81143E+04   -1.06217E+02    6.12848E-01    1.22855E-01   -1.20692E-04       3
 6.46194E-08   -1.40387E-11   -3.09649E+04    3.65169E+01                      4
R205C7H13O4H2           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
-3.41691E+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
R206C7H14OOOOH          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
R207C4H9OO              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
-1.64981E+04   -5.72510E+01   -1.15391E-01    6.30619E-02   -4.71494E-05       3
 1.63007E-08   -1.48274E-12   -1.17259E+04    2.93080E+01                      4
R208C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 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   -2.54055E+04    1.05551E+01                      4
R209C7H13O4H2           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   -2.54055E+04    1.05551E+01                      4
R210C7H13O4H2           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
-3.15215E+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
R211C7H13O4H2           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
-3.54058E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94436E+04    1.19254E+01                      4
R212C5H10OOOOH          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   -8.14626E+01    6.74655E+00    4.96086E-02    1.51304E-05       3
-5.37340E-08    2.37228E-11   -2.55589E+04    6.93703E+00                      4
R213C5H11OO             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
-1.97347E+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
R214C5H10OOH            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
-1.33136E+04   -6.07627E+01    6.00935E+00    4.10908E-02    1.53302E-05       3
-4.62069E-08    2.00942E-11   -9.27332E+03    6.81659E+00                      4
R215C7H13O4H2           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
-3.54058E+04   -9.80413E+01    6.51363E+00    8.25618E-02   -3.15269E-05       3
-1.70330E-08    1.25696E-11   -2.94436E+04    1.19254E+01                      4
R216C7H13O4H2           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
-3.15215E+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
R217C7H13O4H2           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
-3.15215E+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
R218C7H13O4H2           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
-3.15215E+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
R219C7H14OOOOH          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   -3.14186E+04    9.78564E+00                      4
R220C7H13O4H2           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
-3.80584E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10553E+04    3.26031E+01                      4
R221C7H13O4H2           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
-3.38256E+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
R222C7H13O4H2           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
-3.38256E+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
R223C7H13O4H2           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
-3.80584E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10553E+04    3.26031E+01                      4
R224C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.95172E+01    3.22772E-02   -9.03418E-06    1.24334E-09   -6.86089E-14       2
-3.38256E+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
R225C7H13O4H2           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
-3.80584E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10553E+04    3.26031E+01                      4
R226C7H14OOOOH          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   -3.76252E+04    1.92965E+01                      4
R227C3H7OO              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
-1.29086E+04   -4.79776E+01   -1.26900E-01    5.26375E-02   -4.34523E-05       3
 1.82031E-08   -2.85659E-12   -8.79556E+03    2.68651E+01                      4
R228C7H13O4H2           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
-3.52346E+04   -1.09960E+02    1.32940E+00    1.15931E-01   -9.90039E-05       3
 4.16135E-08   -5.94711E-12   -2.78005E+04    3.40991E+01                      4
R229C7H13O4H2           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   -2.69003E+04    3.62018E+01                      4
R230C7H13O4H2           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   -2.69003E+04    3.55087E+01                      4
R231C7H13O4H2           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
-3.80584E+04   -1.04877E+02    1.55211E+00    1.16192E-01   -1.05858E-04       3
 5.11612E-08   -9.63226E-12   -3.10553E+04    3.26031E+01                      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
-3.46642E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85846E+04    1.01360E+01                      4
R233C7H13O4H2           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
-3.14538E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55056E+04    6.26062E+00                      4
R234C7H14OOOOH          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
-3.79003E+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
R235C7H14OOOOH          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
-3.59007E+04   -9.99421E+01    2.87463E+00    9.63752E-02   -5.64548E-05       3
 6.80405E-09    4.08129E-12   -2.88310E+04    2.75332E+01                      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
-3.46642E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85846E+04    1.01360E+01                      4
R237C7H13O4H2           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
-3.14538E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55056E+04    6.26062E+00                      4
R238C7H13O4H2           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
-3.11340E+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
R239C7H13O4H2           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
-3.14538E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55056E+04    6.26062E+00                      4
R240C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.81843E+01    3.36700E-02   -9.53959E-06    1.32437E-09   -7.35122E-14       2
-3.11340E+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
R241C7H13O4H2           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
-3.46642E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85846E+04    1.01360E+01                      4
R242C7H14OOOOH          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
-4.09343E+04   -1.02242E+02    3.82351E+00    7.91990E-02   -2.82992E-06       3
-5.28530E-08    2.59241E-11   -3.38395E+04    2.30989E+01                      4
R243C7H13O4H2           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
-3.14538E+04   -9.84055E+01    8.00428E+00    7.10725E-02   -2.66111E-06       3
-4.50996E-08    2.21017E-11   -2.55056E+04    6.26062E+00                      4
R244C7H13O4H2           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
-3.11340E+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
R245C7H13O4H2           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
-3.46642E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85846E+04    1.01360E+01                      4
R246C5H10OOOOH          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
-3.07599E+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
R247C5H10OOOOH          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   -8.21554E+01    6.83506E+00    4.89942E-02    1.66070E-05       3
-5.52080E-08    2.42443E-11   -2.55684E+04    5.86989E+00                      4
R248C5H10OOOOH          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   -8.21540E+01    6.81264E+00    4.91504E-02    1.62312E-05       3
-5.48328E-08    2.41115E-11   -2.55660E+04    5.96597E+00                      4
R249C5H10OOOOH          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
-2.88053E+04   -8.12487E+01    3.01512E+00    7.43746E-02   -4.62199E-05       3
 7.66715E-09    2.41829E-12   -2.29878E+04    2.33489E+01                      4
R250C5H10OOH            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
-1.33263E+04   -6.14952E+01    5.09002E+00    4.76127E-02    8.43541E-07       3
-3.31039E-08    1.58162E-11   -9.18496E+03    1.06463E+01                      4
R251C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20923E+01    3.76158E-02   -1.07842E-05    1.50980E-09   -8.42834E-14       2
-3.65680E+04   -1.26444E+02    8.91329E-01    1.23082E-01   -8.78415E-05       3
 2.30256E-08    1.20655E-12   -2.80512E+04    3.46530E+01                      4
R252C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17941E+01    3.75107E-02   -1.06549E-05    1.47662E-09   -8.15658E-14       2
-4.00410E+04   -1.23811E+02    6.02050E-01    1.26021E-01   -9.77566E-05       3
 3.38764E-08   -2.67879E-12   -3.16506E+04    3.65462E+01                      4
R253C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17606E+01    3.75968E-02   -1.07120E-05    1.49081E-09   -8.27586E-14       2
-3.68528E+04   -1.24310E+02    7.39333E-01    1.25110E-01   -9.53778E-05       3
 3.13447E-08   -1.74429E-12   -2.84972E+04    3.52610E+01                      4
R254C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.09437E+01    3.85164E-02   -1.10673E-05    1.55137E-09   -8.66474E-14       2
-3.85508E+04   -1.20228E+02    2.78944E+00    1.11538E-01   -6.77216E-05       3
 7.17915E-09    6.10448E-12   -3.06680E+04    2.61359E+01                      4
R255C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20408E+01    3.77085E-02   -1.08393E-05    1.52298E-09   -8.53765E-14       2
-3.78563E+04   -1.25465E+02    1.11072E+00    1.21555E-01   -8.41632E-05       3
 1.93435E-08    2.51276E-12   -2.93830E+04    3.44177E+01                      4
R256C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
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 3.10304E+01    3.86064E-02   -1.11232E-05    1.56165E-09   -8.72809E-14       2
-4.01259E+04   -1.20761E+02    6.53997E+00    8.66547E-02   -6.12155E-06       3
-5.44439E-08    2.74796E-11   -3.28388E+04    9.64038E+00                      4
R257C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.21979E+01    3.76721E-02   -1.08203E-05    1.51544E-09   -8.45384E-14       2
-3.94595E+04   -1.26391E+02    5.00257E+00    9.57037E-02   -2.02687E-05       3
-4.45413E-08    2.46793E-11   -3.15692E+04    1.73219E+01                      4
R258C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.21884E+01    3.76888E-02   -1.08303E-05    1.51787E-09   -8.47446E-14       2
-3.81472E+04   -1.26337E+02    4.94206E+00    9.61076E-02   -2.12041E-05       3
-4.36363E-08    2.43672E-11   -3.02541E+04    1.75805E+01                      4
R259C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17521E+01    3.78324E-02   -1.08485E-05    1.51984E-09   -8.49328E-14       2
-4.15661E+04   -1.24324E+02    5.00138E+00    9.66426E-02   -2.53767E-05       3
-3.84884E-08    2.24913E-11   -3.38909E+04    1.66092E+01                      4
R260C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.23770E+01    3.75697E-02   -1.08167E-05    1.52112E-09   -8.52986E-14       2
-3.98323E+04   -1.28584E+02    4.33538E+00    1.02663E-01   -3.81557E-05       3
-2.68183E-08    1.86224E-11   -3.18807E+04    1.84674E+01                      4
R261C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20011E+01    3.76326E-02   -1.07942E-05    1.51421E-09   -8.47886E-14       2
-4.00999E+04   -1.26898E+02    4.07790E+00    1.05411E-01   -4.73961E-05       3
-1.68233E-08    1.50866E-11   -3.23153E+04    1.88305E+01                      4
R262C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.23974E+01    3.75321E-02   -1.07938E-05    1.51555E-09   -8.48294E-14       2
-3.98407E+04   -1.28698E+02    4.66500E+00    1.00374E-01   -3.26547E-05       3
-3.23097E-08    2.05654E-11   -3.19160E+04    1.70719E+01                      4
R263C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.19010E+01    3.77826E-02   -1.08750E-05    1.53252E-09   -8.62569E-14       2
-4.32344E+04   -1.26347E+02    4.08466E+00    1.05335E-01   -4.74309E-05       3
-1.66036E-08    1.49613E-11   -3.54842E+04    1.88111E+01                      4
R264C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12338E+01    3.84888E-02   -1.10851E-05    1.55450E-09   -8.67385E-14       2
-4.78265E+04   -1.26954E+02    1.98140E+00    9.66035E-02   -6.89892E-06       3
-6.36719E-08    3.21665E-11   -3.91708E+04    2.85857E+01                      4
R265C4H8OOOOH           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
-2.96276E+04   -7.74386E+01    5.63013E+00    4.69489E-02    2.61001E-06       3
-3.77523E-08    1.79632E-11   -2.48064E+04    6.50062E+00                      4
R266C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.11628E+01    3.80892E-02   -1.08785E-05    1.51759E-09   -8.44419E-14       2
-3.85891E+04   -1.20647E+02    1.31160E+00    1.21926E-01   -9.14768E-05       3
 2.95172E-08   -1.43680E-12   -3.05197E+04    3.30251E+01                      4
R267C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20618E+01    3.76679E-02   -1.08138E-05    1.51661E-09   -8.48313E-14       2
-3.78637E+04   -1.25580E+02    9.35824E-01    1.22766E-01   -8.70684E-05       3
 2.22425E-08    1.48658E-12   -2.93643E+04    3.51587E+01                      4
R268C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17188E+01    3.76723E-02   -1.07570E-05    1.50160E-09   -8.36563E-14       2
-3.68367E+04   -1.23386E+02    9.74505E-01    1.23455E-01   -9.13512E-05       3
 2.72813E-08   -2.93413E-13   -2.85220E+04    3.49615E+01                      4
R269C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20923E+01    3.76158E-02   -1.07842E-05    1.50980E-09   -8.42834E-14       2
-3.65680E+04   -1.25058E+02    8.91329E-01    1.23082E-01   -8.78415E-05       3
 2.30256E-08    1.20655E-12   -2.80512E+04    3.60392E+01                      4
R270C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17941E+01    3.75107E-02   -1.06549E-05    1.47662E-09   -8.15658E-14       2
-4.00410E+04   -1.23811E+02    6.02050E-01    1.26021E-01   -9.77566E-05       3
 3.38764E-08   -2.67879E-12   -3.16506E+04    3.65462E+01                      4
R271C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.44619E+01    2.28303E-02   -6.18017E-06    8.30684E-10   -4.51231E-14       2
-3.17414E+04   -9.30833E+01    1.25560E+00    8.28516E-02   -5.35696E-05       3
 7.45168E-09    3.91131E-12   -2.51958E+04    2.76976E+01                      4
R272C4H8OOOOH           C   4H   9O   4     G  0300.00   5000.00  1000.00      1
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 2.09064E+01    1.83898E-02   -4.75218E-06    6.15368E-10   -3.24599E-14       2
-2.63305E+04   -7.27616E+01    1.88363E+00    6.94733E-02   -5.21490E-05       3
 1.71674E-08   -1.25214E-12   -2.09446E+04    2.60456E+01                      4
R273C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.37437E+01    3.60876E-02   -1.02463E-05    1.42324E-09   -7.89486E-14       2
-4.25296E+04   -1.37789E+02   -9.44604E-01    1.38719E-01   -1.17364E-04       3
 4.51620E-08   -4.66235E-12   -3.34692E+04    3.93228E+01                      4
R274C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.30314E+01    3.61676E-02   -1.01800E-05    1.40473E-09   -7.75426E-14       2
-4.66983E+04   -1.34475E+02   -1.75821E+00    1.46323E-01   -1.40702E-04       3
 6.98312E-08   -1.33477E-11   -3.79317E+04    4.14575E+01                      4
R275C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.37416E+01    3.60921E-02   -1.02495E-05    1.42411E-09   -7.90286E-14       2
-4.25282E+04   -1.37370E+02   -1.34210E+00    1.41486E-01   -1.24032E-04       3
 5.18381E-08   -7.03121E-12   -3.34268E+04    4.14102E+01                      4
R276C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.11809E+01    3.83023E-02   -1.10074E-05    1.54533E-09   -8.65229E-14       2
-4.01382E+04   -1.21900E+02    5.86827E+00    9.14702E-02   -1.65383E-05       3
-4.53744E-08    2.46195E-11   -3.27771E+04    1.20145E+01                      4
R277C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.21847E+01    3.76970E-02   -1.08359E-05    1.51931E-09   -8.48710E-14       2
-3.94543E+04   -1.27416E+02    4.89092E+00    9.64770E-02   -2.21244E-05       3
-4.26897E-08    2.40242E-11   -3.15572E+04    1.66964E+01                      4
R278C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.14931E+01    3.77390E-02   -1.07467E-05    1.49549E-09   -8.30419E-14       2
-4.23231E+04   -1.23524E+02    4.29729E+00    1.02551E-01   -4.17785E-05       3
-2.17065E-08    1.66453E-11   -3.47348E+04    1.85932E+01                      4
R279C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.22107E+01    3.76495E-02   -1.08074E-05    1.51252E-09   -8.43100E-14       2
-3.81562E+04   -1.26462E+02    5.04173E+00    9.54155E-02   -1.95405E-05       3
-4.52961E-08    2.49538E-11   -3.02647E+04    1.71585E+01                      4
R280C5H10OOOOH          C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.44420E+01    2.20011E-02   -5.75357E-06    7.49675E-10   -3.96076E-14       2
-3.67485E+04   -9.60720E+01    2.29002E+00    6.50907E-02    1.43622E-06       3
-5.35599E-08    2.62252E-11   -3.02135E+04    2.18007E+01                      4
R281C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.14980E+01    3.77305E-02   -1.07418E-05    1.49436E-09   -8.29482E-14       2
-4.23255E+04   -1.23147E+02    4.51312E+00    1.01045E-01   -3.81366E-05       3
-2.53613E-08    1.79447E-11   -3.47577E+04    1.80860E+01                      4
R282C4H8OOOOH           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
-3.13150E+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
R283C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.23770E+01    3.75697E-02   -1.08167E-05    1.52112E-09   -8.52986E-14       2
-4.02348E+04   -1.29682E+02    4.33538E+00    1.02663E-01   -3.81557E-05       3
-2.68183E-08    1.86224E-11   -3.22833E+04    1.73689E+01                      4
R284C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.21149E+01    3.74270E-02   -1.06717E-05    1.48490E-09   -8.23562E-14       2
-4.05476E+04   -1.27937E+02    4.14755E+00    1.04932E-01   -4.62541E-05       3
-1.79571E-08    1.54863E-11   -3.27254E+04    1.81295E+01                      4
R285C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.23274E+01    3.76572E-02   -1.08676E-05    1.53304E-09   -8.62701E-14       2
-4.02151E+04   -1.28308E+02    4.52831E+00    1.01334E-01   -3.49895E-05       3
-2.99564E-08    1.97261E-11   -3.23041E+04    1.76489E+01                      4
R286C4H8OOOOH           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
R287C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.19010E+01    3.77826E-02   -1.08750E-05    1.53252E-09   -8.62569E-14       2
-4.36370E+04   -1.26752E+02    4.08466E+00    1.05335E-01   -4.74309E-05       3
-1.66036E-08    1.49613E-11   -3.58868E+04    1.84057E+01                      4
R288C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
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 3.14371E+01    3.75664E-02   -1.06346E-05    1.47088E-09   -8.11749E-14       2
-3.82485E+04   -1.23861E+02    4.11729E-01    1.28326E-01   -1.05700E-04       3
 4.23820E-08   -5.63759E-12   -3.00311E+04    3.49790E+01                      4
R289C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.16504E+01    3.77663E-02   -1.08050E-05    1.51213E-09   -8.44848E-14       2
-3.95811E+04   -1.24109E+02    8.05423E-01    1.24618E-01   -9.44069E-05       3
 3.05508E-08   -1.50752E-12   -3.12699E+04    3.45853E+01                      4
R290C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.18118E+01    3.75070E-02   -1.06600E-05    1.47867E-09   -8.17736E-14       2
-3.64710E+04   -1.25695E+02    7.12992E-01    1.25266E-01   -9.56913E-05       3
 3.16037E-08   -1.81977E-12   -2.80914E+04    3.42778E+01                      4
R291C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.21333E+01    3.75417E-02   -1.07401E-05    1.49928E-09   -8.34137E-14       2
-3.61817E+04   -1.26672E+02    9.96693E-01    1.22350E-01   -8.60837E-05       3
 2.12732E-08    1.82517E-12   -2.76599E+04    3.42070E+01                      4
R292C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.17521E+01    3.78324E-02   -1.08485E-05    1.51984E-09   -8.49328E-14       2
-4.15661E+04   -1.24730E+02    5.00138E+00    9.66426E-02   -2.53767E-05       3
-3.84884E-08    2.24913E-11   -3.38909E+04    1.62038E+01                      4
R293C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.16488E+01    3.77678E-02   -1.08052E-05    1.51203E-09   -8.44677E-14       2
-3.99825E+04   -1.23000E+02    7.12873E-01    1.25243E-01   -9.58667E-05       3
 3.19737E-08   -2.00093E-12   -3.16623E+04    3.60783E+01                      4
R294C8H16OOOOH          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.12338E+01    3.84888E-02   -1.10851E-05    1.55450E-09   -8.67385E-14       2
-4.78264E+04   -1.27359E+02    1.98140E+00    9.66035E-02   -6.89892E-06       3
-6.36719E-08    3.21665E-11   -3.91708E+04    2.81803E+01                      4
R295C3H5O4H2            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
-2.12814E+04   -5.95781E+01    2.79513E+00    6.52872E-02   -7.36435E-05       3
 4.50951E-08   -1.12080E-11   -1.73094E+04    2.06618E+01                      4
R296C4H7O4H2            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
-2.49690E+04   -7.15394E+01    1.72784E+00    8.33471E-02   -9.45224E-05       3
 5.90079E-08   -1.50802E-11   -2.01344E+04    2.69143E+01                      4
R297C4H7O4H2            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
-2.49360E+04   -7.05352E+01    2.85042E+00    7.54180E-02   -7.66630E-05       3
 4.25471E-08   -9.61697E-12   -2.02445E+04    2.22234E+01                      4
R298C4H7O4H2            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
-2.37192E+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
R299C4H7O4H2            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
R300C4H7O4H2            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
R301C5H9O4H2            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
-2.75185E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27013E+04    7.52925E+00                      4
R302C5H9O4H2            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
R303C7H13O4H2           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
-3.75522E+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
R304C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 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
R305C7H13O4H2           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   -3.10405E+04    1.97604E+01                      4
R306C5H9O4H2            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
-2.82412E+04   -7.83263E+01    6.81537E+00    5.94061E-02   -1.84344E-05       3
-1.90940E-08    1.19627E-11   -2.36171E+04    7.06306E+00                      4
R307C5H9O4H2            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
-2.43626E+04   -8.02932E+01    6.77455E+00    5.86963E-02   -1.43078E-05       3
-2.38039E-08    1.35825E-11   -1.95254E+04    7.81866E+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   -1.96296E+04    3.36332E+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
R310C5H10OOOOH          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   -8.93308E+01    9.67386E-01    8.90932E-02   -7.21982E-05       3
 2.62090E-08   -2.32611E-12   -2.70936E+04    3.10109E+01                      4
R311C5H10OOOOH          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
R312C5H10OOH            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
-1.71917E+04   -5.88004E+01    5.77216E+00    4.37225E-02    6.60286E-06       3
-3.69192E-08    1.68589E-11   -1.33352E+04    7.23922E+00                      4
R313C4H7O4H2            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
-2.44502E+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
R314C5H9O4H2            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
-2.73441E+04   -8.09663E+01    3.78815E+00    6.76840E-02   -2.53542E-05       3
-1.87781E-08    1.29695E-11   -2.19407E+04    2.06610E+01                      4
R315C5H9O4H2            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
-2.73441E+04   -8.09663E+01    3.78815E+00    6.76840E-02   -2.53542E-05       3
-1.87781E-08    1.29695E-11   -2.19407E+04    2.06610E+01                      4
R316C5H9O4H2            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
-2.73171E+04   -8.00343E+01    5.14353E+00    5.81283E-02   -3.56054E-06       3
-3.91896E-08    1.98379E-11   -2.20755E+04    1.49860E+01                      4
R317C5H9O4H2            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   -8.30807E+01    4.35484E+00    6.27947E-02   -1.09825E-05       3
-3.38834E-08    1.83099E-11   -2.14386E+04    1.82948E+01                      4
R318C5H9O4H2            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
-2.75185E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27013E+04    7.52925E+00                      4
R319C3H5O4H2            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
-2.02106E+04   -6.02783E+01    2.34223E+00    5.60746E-02   -3.97539E-05       3
 6.18067E-09    3.11385E-12   -1.59124E+04    2.33135E+01                      4
R320C3H5O4H2            C   3H   7O   4     G  0300.00   5000.00  1000.00      1
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 1.91034E+01    1.11754E-02   -2.38254E-06    2.67780E-10   -1.28299E-14       2
-7.37253E+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
R321C7H13O4H2           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   -3.16833E+04    1.62181E+01                      4
R322C7H13O4H2           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
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
-3.75522E+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
 2.54793E+01    3.76842E-02   -1.12157E-05    1.61716E-09   -9.23677E-14       2
-3.75522E+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
R325C7H13O4H2           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   -3.16833E+04    1.62181E+01                      4
R326C7H13O4H2           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   -3.10405E+04    1.97604E+01                      4
R327C4H8OOH             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
-1.00667E+04   -5.43474E+01    9.20577E-01    6.50158E-02   -6.06391E-05       3
 3.16774E-08   -6.83465E-12   -5.79018E+03    2.66741E+01                      4
R328C4H9                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
 4.66951E+03   -1.28601E+01    2.59734E-01    4.63002E-02   -3.08637E-05       3
 1.04408E-08   -9.04074E-13    6.56021E+03    2.51000E+01                      4
R329C5H9O4H2            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
-2.43764E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95191E+04    8.06816E+00                      4
R330C5H9O4H2            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
-2.82412E+04   -7.83263E+01    6.81537E+00    5.94061E-02   -1.84344E-05       3
-1.90940E-08    1.19627E-11   -2.36171E+04    7.06306E+00                      4
R331C5H9O4H2            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   -1.96296E+04    3.36332E+00                      4
R332C5H9O4H2            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
R333C5H11               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
 2.27837E+03   -8.15961E+00   -6.61971E-01    6.31951E-02   -4.86146E-05       3
 2.06999E-08   -3.22505E-12    3.76775E+03    2.99721E+01                      4
R334C5H10OOOOH          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   -9.00238E+01    9.67386E-01    8.90932E-02   -7.21982E-05       3
 2.62090E-08   -2.32611E-12   -2.70936E+04    3.03178E+01                      4
R335C7H13O4H2           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
-3.11340E+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
R336C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 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   -2.54055E+04    1.05551E+01                      4
R337C7H13O4H2           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   -2.54055E+04    1.05551E+01                      4
R338C7H13O4H2           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
-3.15215E+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
R339C7H13O4H2           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
-3.15215E+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
R340C5H9O4H2            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
R341C5H9O4H2            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
R342C5H9O4H2            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
-2.75185E+04   -8.00375E+01    6.84467E+00    5.81915E-02   -1.33377E-05       3
-2.45682E-08    1.38002E-11   -2.27013E+04    7.52925E+00                      4
R343C7H13O4H2           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
-3.73185E+04   -9.39268E+01    4.66844E+00    8.09014E-02   -8.86140E-06       3
-4.80859E-08    2.52381E-11   -3.11691E+04    1.86525E+01                      4
R344C7H13O4H2           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
-3.75642E+04   -9.12539E+01    4.36718E+00    8.39519E-02   -1.88235E-05       3
-3.73730E-08    2.14488E-11   -3.15989E+04    1.98943E+01                      4
R345C7H13O4H2           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
-3.75522E+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
R346C7H13O4H2           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
-3.75522E+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
R347C7H13O4H2           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   -3.16833E+04    1.62181E+01                      4
R348C3H7                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
 9.45583E+03    9.26810E+00    1.12279E+00    2.81622E-02   -7.69315E-06       3
-7.36009E-09    4.81993E-12    9.72798E+03    1.91610E+01                      4
R349C7H13O4H2           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
-3.25432E+04   -1.02025E+02    7.21867E+00    7.57093E-02   -9.99194E-06       3
-3.99029E-08    2.06183E-11   -2.62779E+04    9.55752E+00                      4
R350C7H13O4H2           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
-2.95368E+04   -9.92811E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28177E+04    2.76165E+01                      4
R351C7H13O4H2           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
-2.95368E+04   -9.92811E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28177E+04    2.76165E+01                      4
R352C7H13O4H2           C   7H  15O   4     G  0300.00   5000.00  1000.00      1
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 2.77519E+01    3.35893E-02   -9.42966E-06    1.29943E-09   -7.17043E-14       2
-2.95368E+04   -9.99742E+01    3.09117E+00    1.04161E-01   -8.27800E-05       3
 3.36383E-08   -4.96659E-12   -2.28177E+04    2.69234E+01                      4
R353C5H9O4H2           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
R354C7H13O4H2          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
-3.45408E+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
R355C7H13O4H2          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
R356C7H13O4H2          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
-3.45460E+04   -1.01227E+02    3.96233E+00    8.75251E-02   -3.04537E-05       3
-2.47215E-08    1.64168E-11   -2.78179E+04    2.35098E+01                      4
R357C7H13O4H2          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
-3.45460E+04   -1.01227E+02    3.96233E+00    8.75251E-02   -3.04537E-05       3
-2.47215E-08    1.64168E-11   -2.78179E+04    2.35098E+01                      4
R358C5H9O4H2           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
-2.55054E+04   -7.90064E+01    2.94642E+00    8.40879E-02   -7.73407E-05       3
 3.94239E-08   -8.40356E-12   -2.01119E+04    2.46521E+01                      4
R359C5H9O4H2           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
-2.43764E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95191E+04    8.06816E+00                      4
R360C5H9O4H2           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
-2.43764E+04   -8.04872E+01    6.71546E+00    5.91114E-02   -1.53168E-05       3
-2.27859E-08    1.32188E-11   -1.95191E+04    8.06816E+00                      4
R361C5H9O4H2           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
-2.23706E+04   -7.95531E+01    3.02378E+00    8.35852E-02   -7.59269E-05       3
 3.78415E-08   -7.80083E-12   -1.69520E+04    2.43147E+01                      4
R362C5H9O4H2           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
-2.23706E+04   -8.02462E+01    3.02378E+00    8.35852E-02   -7.59269E-05       3
 3.78415E-08   -7.80083E-12   -1.69520E+04    2.36216E+01                      4
R363C5H10OOOOH         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
-3.34443E+04   -8.93321E+01    9.89811E-01    8.89371E-02   -7.18225E-05       3
 2.58338E-08   -2.19341E-12   -2.70960E+04    3.09148E+01                      4
R364C4H7O4H2           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
-2.16584E+04   -6.91089E+01    2.96955E+00    7.20411E-02   -6.97457E-05       3
 3.74100E-08   -8.32324E-12   -1.69860E+04    2.12430E+01                      4
R365C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.52376E+01    2.12487E-02   -5.52606E-06    7.21427E-10   -3.84125E-14       2
-2.50652E+04   -9.41213E+01    1.70838E+00    8.80352E-02   -7.10043E-05       3
 2.46414E-08   -1.72576E-12   -1.87457E+04    2.68139E+01                      4
R366C5H9O4H2           C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.49386E+01    2.11503E-02   -5.40281E-06    6.89372E-10   -3.57468E-14       2
-2.85390E+04   -9.21800E+01    1.38066E+00    9.12508E-02   -8.16050E-05       3
 3.61937E-08   -5.86374E-12   -2.23411E+04    2.81754E+01                      4
R367C8H15O4H2          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20785E+01    3.67618E-02   -1.03359E-05    1.42449E-09   -7.85358E-14       2
-1.34625E+04   -1.27670E+02    2.07716E+00    1.04270E-01   -3.03091E-05       3
-4.05120E-08    2.44161E-11   -4.97234E+03    2.99058E+01                      4
R368C8H15O4H2          C   8H  17O   4     G  0300.00   5000.00  1000.00      1
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 3.16815E+01    3.68597E-02   -1.03326E-05    1.42173E-09   -7.83364E-14       2
-4.14319E+04   -1.25867E+02    2.10480E+00    1.05033E-01   -3.47649E-05       3
-3.53053E-08    2.25782E-11   -3.31475E+04    2.90625E+01                      4
R369C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.09493E+01    3.76247E-02   -1.05950E-05    1.46015E-09   -8.04004E-14       2
-4.31619E+04   -1.22251E+02    3.47502E+00    9.61793E-02   -1.84406E-05       3
-4.81620E-08    2.64262E-11   -3.52456E+04    2.28165E+01                      4
R370C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20462E+01    3.68161E-02   -1.03660E-05    1.43125E-09   -7.90671E-14       2
-4.24675E+04   -1.27488E+02    2.07716E+00    1.04270E-01   -3.03091E-05       3
-4.05120E-08    2.44161E-11   -3.39910E+04    2.99058E+01                      4
R371C4H7O4H2            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   -1.83352E+04    7.84390E+00                      4
R372C4H7O4H2            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
-2.63589E+04   -7.48902E+01    5.66217E+00    5.59936E-02   -2.69755E-05       3
-7.46451E-09    7.64168E-12   -2.19417E+04    8.06466E+00                      4
R373C4H7O4H2            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
-2.09643E+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
R374C4H7O4H2            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
-2.30774E+04   -7.11202E+01    2.19451E+00    7.65744E-02   -7.70450E-05       3
 4.27577E-08   -9.90658E-12   -1.81096E+04    2.57368E+01                      4
R375C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
 2.51614E+01    2.05281E-02   -5.16654E-06    6.55659E-10   -3.40766E-14       2
-1.00652E+04   -9.57022E+01    2.41485E+00    7.25453E-02   -2.14415E-05       3
-3.09519E-08    1.86762E-11   -3.74242E+03    2.34040E+01                      4
R376C4H7O4H2            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
-2.65962E+04   -6.94546E+01    5.01633E+00    4.70988E-02    1.36562E-06       3
-3.83526E-08    1.88621E-11   -2.21019E+04    1.22221E+01                      4
R377C4H7O4H2            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
-8.48716E+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
R378C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.09911E+01    3.75165E-02   -1.05953E-05    1.47125E-09   -8.18849E-14       2
-4.31308E+04   -1.22785E+02    2.58488E+00    1.02526E-01   -3.25710E-05       3
-3.53573E-08    2.22362E-11   -3.51607E+04    2.61133E+01                      4
R379C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.20462E+01    3.68161E-02   -1.03660E-05    1.43125E-09   -7.90671E-14       2
-1.34491E+04   -1.28587E+02    2.19723E+00    1.03438E-01   -2.83127E-05       3
-4.25030E-08    2.51202E-11   -4.98521E+03    2.82986E+01                      4
R380C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.16236E+01    3.69637E-02   -1.03943E-05    1.43645E-09   -7.95552E-14       2
-4.14085E+04   -1.25949E+02    1.87212E+00    1.06639E-01   -3.86019E-05       3
-3.14936E-08    2.12350E-11   -3.31225E+04    2.96437E+01                      4
R381C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.19529E+01    3.69838E-02   -1.04656E-05    1.45507E-09   -8.10417E-14       2
-4.11220E+04   -1.26968E+02    2.03290E+00    1.04554E-01   -3.09362E-05       3
-3.99351E-08    2.42270E-11   -3.26775E+04    3.00965E+01                      4
R382C4H7O4H2            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
-2.75947E+04   -6.84260E+01    3.52913E+00    5.99555E-02   -3.05055E-05       3
-7.51733E-09    8.35623E-12   -2.30711E+04    1.93804E+01                      4
R383C5H9O4H2            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
-2.70009E+04   -8.69505E+01    2.21088E+00    8.96078E-02   -8.22315E-05       3
 3.81369E-08   -6.45791E-12   -2.11801E+04    2.68063E+01                      4
R384C5H9O4H2            C   5H  11O   4     G  0300.00   5000.00  1000.00      1
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 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
R385C5H9O4H2            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
-2.69962E+04   -8.81277E+01    8.88244E-01    9.89192E-02   -1.03395E-04       3
 5.78785E-08   -1.30759E-11   -2.10485E+04    3.16519E+01                      4
R386C5H9O4H2            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
-3.08780E+04   -8.49714E+01    1.75572E+00    9.37524E-02   -9.45938E-05       3
 5.10513E-08   -1.09758E-11   -2.52187E+04    2.81518E+01                      4
R387C5H9O4H2            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
-2.81770E+04   -7.68845E+01    7.50795E+00    5.44625E-02   -7.75087E-06       3
-2.83911E-08    1.48911E-11   -2.36813E+04    4.19279E+00                      4
R388C5H10OOOOH          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   -7.32991E+01    3.98808E+00    5.62495E-02    1.27706E-05       3
-5.84226E-08    2.71022E-11   -3.17362E+04    1.69133E+01                      4
R389C4H8OOOOH           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
-2.98132E+04   -7.94808E+01    1.09802E+00    7.76655E-02   -6.60467E-05       3
 2.56165E-08   -2.80149E-12   -2.41783E+04    2.79707E+01                      4
R390C5H9O4H2            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
-3.12296E+04   -7.90957E+01    3.73250E+00    6.90649E-02   -3.10979E-05       3
-1.24488E-08    1.07748E-11   -2.60221E+04    2.03137E+01                      4
R391C3H5O4H2            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
-2.41100E+04   -5.91275E+01    1.03312E+00    6.63010E-02   -6.55796E-05       3
 3.12088E-08   -5.34218E-12   -1.98699E+04    2.82100E+01                      4
R392C4H7O4H2            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
-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
R393C5H9O4H2            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
R394C5H9O4H2            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
-3.09080E+04   -8.59370E+01    6.25781E-01    1.01744E-01   -1.12632E-04       3
 6.77164E-08   -1.65192E-11   -2.51080E+04    3.28721E+01                      4
R395C7H13O4H2           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
-3.53780E+04   -9.70818E+01    8.02255E+00    7.19328E-02   -7.13493E-06       3
-4.00558E-08    2.03676E-11   -2.95948E+04    5.60133E+00                      4
R396C7H13O4H2           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
-3.46642E+04   -9.94696E+01    7.07605E+00    7.76349E-02   -1.74815E-05       3
-3.14652E-08    1.75845E-11   -2.85846E+04    1.01360E+01                      4
R397C5H9O4H2            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
-3.08780E+04   -8.49714E+01    1.75572E+00    9.37524E-02   -9.45938E-05       3
 5.10513E-08   -1.09758E-11   -2.52187E+04    2.81518E+01                      4
R398C7H13O4H2           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   -3.10405E+04    1.97604E+01                      4
R399C3H5O4H2            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
-2.35073E+04   -6.02984E+01   -1.66210E+00    8.16867E-02   -9.24917E-05       3
 5.32469E-08   -1.17222E-11   -1.87632E+04    3.84113E+01                      4
R400C4H7O4H2            C   4H   9O   4     G  0300.00   5000.00  1000.00      1
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 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
R401C7H13O4H2           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
-3.26727E+04   -9.87512E+01    2.91224E+00    1.05372E-01   -8.59036E-05       3
 3.69365E-08   -6.17956E-12   -2.59668E+04    2.83836E+01                      4
R402C7H13O4H2           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
-3.44804E+04   -9.97477E+01    5.11624E+00    7.93626E-02   -1.19959E-05       3
-4.18140E-08    2.21141E-11   -2.79312E+04    1.86886E+01                      4
R403C7H13O4H2           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
R404C7H13O4H2           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
-3.83978E+04   -9.88988E+01    3.75694E+00    8.99359E-02   -3.86506E-05       3
-1.59634E-08    1.33690E-11   -3.18832E+04    2.37978E+01                      4
R405C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.14424E+01    3.67056E-02   -1.01891E-05    1.38670E-09   -7.55248E-14       2
-4.53724E+04   -1.24781E+02    1.49931E+00    1.10231E-01   -4.96806E-05       3
-1.98205E-08    1.71440E-11   -3.71702E+04    3.10432E+01                      4
R406C8H15O4H2           C   8H  17O   4     G  0300.00   5000.00  1000.00      1
 3.14424E+01    3.67056E-02   -1.01891E-05    1.38670E-09   -7.55248E-14       2
-4.53724E+04   -1.25186E+02    1.49931E+00    1.10231E-01   -4.96806E-05       3
-1.98205E-08    1.71440E-11   -3.71702E+04    3.06378E+01                      4
R407C5H9O4H2            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
R408C5H9O4H2            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   -2.51991E+04    1.54913E+01                      4
R409C5H9O4H2            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   -2.57179E+04    1.71908E+01                      4
R410C4H7O4H2            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
-2.72625E+04   -7.46057E+01    1.77139E+00    8.31258E-02   -9.03749E-05       3
 5.23949E-08   -1.21385E-11   -2.22912E+04    2.62909E+01                      4
R411C4H8OOOOH           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
-3.33034E+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
R412C5H10OOOOH          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
-3.68286E+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
R413C5H9O4H2            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   -2.58115E+04    1.31552E+01                      4
R414C3H6OOOOH           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
-3.01604E+04   -5.89553E+01   -1.98923E+00    7.56273E-02   -7.29458E-05       3
 3.39464E-08   -5.33789E-12   -2.52267E+04    3.87648E+01                      4
R415C4H7O4H2            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
-2.68700E+04   -6.19722E+01    5.14911E+00    4.68057E-02    5.39174E-06       3
-4.36390E-08    2.12905E-11   -2.28846E+04    1.12667E+01                      4
R416C4H8OOH             C   4H   9O   2     G  0300.00   5000.00  1000.00      1
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 1.63522E+01    1.74212E-02   -4.48514E-06    5.80325E-10   -3.06582E-14       2
-1.39465E+04   -5.24021E+01    6.08161E-01    6.81720E-02   -7.06320E-05       3
 4.22312E-08   -1.05184E-11   -9.84410E+03    2.74149E+01                      4
R417C5H10OOH           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
-1.72480E+04   -6.08382E+01    4.62608E+00    5.18306E-02   -1.17247E-05       3
-1.99563E-08    1.12071E-11   -1.32228E+04    1.13342E+01                      4
R418C3H6OOH            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
-1.03160E+04   -4.19655E+01    1.87135E+00    4.87528E-02   -4.64913E-05       3
 2.50715E-08   -5.50182E-12   -7.04004E+03    1.96369E+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
.C7H13Y                C   7H  13O   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
.C8H15Y                C   8H  15O   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
 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
.COC7H15               C   8H  15O   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
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 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
.COOOC7H15             C   8H  15O   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
.C8H15O#4              C   8H  15O   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
.C8H15O#5              C   8H  15O   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
.C8H15O#6              C   8H  15O   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
 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
.OOC8H15O#4            C   8H  15O   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
.OOC8H15O#5            C   8H  15O   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
.OOC8H15O#6            C   8H  15O   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
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 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
 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
.C8H14O#4OOH            C   8H  15O   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
.C8H14O#5OOH            C   8H  15O   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
.C8H14O#6OOH            C   8H  15O   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
.OOC8H14O#4OOH          C   8H  15O   5     G  0300.00   5000.00  1000.00      1
```

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 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
.OOC8H14O#5OOH          C   8H  15O   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
.OOC8H14O#6OOH          C   8H  15O   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
END

REACTIONS

!     -----------------
!     PRIMARY REACTIONS
!     -----------------
!   unimolecular initiations :
C7H16=>R19C3H7+R20C4H9    8.8E+16  0.0  86591.6  ! UI 1 KB
C7H16=>R11C2H5+R35C5H11    7.6E+16  0.0  85570.3  ! UI 2 KB
C7H16=>R4CH3+RC6H13    1.4E+17  0.0  86952.7  ! UI 3 KB
C8H18=>R4CH3+R1C7H15    5.8E+17  0.0  83384.9  ! UI 1 KB
C8H18=>R37C4H9+R40C4H9    7.1E+16  0.0  79273.7  ! UI 2 KB
C8H18=>R348C3H7+R42C5H11    1.1E+17  0.0  84342.3  ! UI 3 KB
C8H18=>R4CH3+R2C7H15    2.6E+17  0.0  87164.3  ! UI 4 KB

R1C7H15=>R19C3H7+C4H8Y    2.0E+13  0.0  28700.0  ! DE 462 CW
R2C7H15=>R37C4H9+C3H6Y    2.0E+13  0.0  28700.0  ! DE 470 CW
RC6H13=>R20C4H9+C2H4Z    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
C8H18+O2=>R3O2H+R25C8H17    3.8E+13  0.0  49000.0  ! BI 5 CN
C8H18+O2=>R3O2H+R26C8H17    2.0E+12  0.0  48000.0  ! BI 6 CN
C8H18+O2=>R3O2H+R27C8H17    2.0E+12  0.0  46000.0  ! BI 7 CN
C8H18+O2=>R3O2H+R28C8H17    2.5E+13  0.0  49000.0  ! BI 8 CN

!   additions :

!   additions with oxygen:
R19C3H7+O2=R29C3H7OO    2.2E+19  -2.5  0.0  ! ADO 9 CN
R20C4H9+O2=R30C4H9OO    2.2E+19  -2.5  0.0  ! ADO 10 CN
R21C7H15+O2=R31C7H15OO    2.2E+19  -2.5  0.0  ! ADO 11 CN
R22C7H15+O2=R32C7H15OO    2.2E+19  -2.5  0.0  ! ADO 12 CN
R23C7H15+O2=R33C7H15OO    2.2E+19  -2.5  0.0  ! ADO 13 CN
R24C7H15+O2=R34C7H15OO    2.2E+19  -2.5  0.0  ! ADO 14 CN
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R25C8H17+O2=R36C8H17OO    2.2E+19  -2.5  0.0  ! ADO 15 CN
R26C8H17+O2=R38C8H17OO    2.2E+19  -2.5  0.0  ! ADO 16 CN
R27C8H17+O2=R39C8H17OO    2.2E+19  -2.5  0.0  ! ADO 17 CN
R28C8H17+O2=R41C8H17OO    2.2E+19  -2.5  0.0  ! ADO 18 CN
R35C5H11+O2=R66C5H11OO    2.2E+19  -2.5  0.0  ! ADO 19 CN
R37C4H9+O2=R72C4H9OO    2.2E+19  -2.5  0.0  ! ADO 20 CN
R40C4H9+O2=R79C4H9OO    2.2E+19  -2.5  0.0  ! ADO 21 CN
R42C5H11+O2=R84C5H11OO    2.2E+19  -2.5  0.0  ! ADO 22 CN
R43C3H6OOH+O2=R85C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 23 CN
R44C3H6OOH+O2=R86C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 24 CN
R45C4H8OOH+O2=R87C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 25 CN
R46C4H8OOH+O2=R88C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 26 CN
R47C4H8OOH+O2=R89C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 27 CN
R48C7H14OOH+O2=R91C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 28 CN
R49C7H14OOH+O2=R92C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 29 CN
R50C7H14OOH+O2=R93C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 30 CN
R51C7H14OOH+O2=R96C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 31 CN
R52C7H14OOH+O2=R97C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 32 CN
R53C7H14OOH+O2=R99C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 33 CN
R54C7H14OOH+O2=R100C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 34 CN
R55C7H14OOH+O2=R102C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 35 CN
R56C7H14OOH+O2=R105C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 36 CN
R57C7H14OOH+O2=R107C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 37 CN
R58C7H14OOH+O2=R109C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 38 CN
R59C7H14OOH+O2=R110C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 39 CN
R60C7H14OOH+O2=R111C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 40 CN
R61C7H14OOH+O2=R114C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 41 CN
R62C7H14OOH+O2=R116C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 42 CN
R63C7H14OOH+O2=R119C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 43 CN
R64C7H14OOH+O2=R120C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 44 CN
R65C7H14OOH+O2=R122C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 45 CN
R67C5H11+O2=R127C5H11OO    2.2E+19  -2.5  0.0  ! ADO 46 CN
R68C8H16OOH+O2=R128C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 47 CN
R69C8H16OOH+O2=R129C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 48 CN
R70C8H16OOH+O2=R130C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 49 CN
R71C8H16OOH+O2=R133C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 50 CN
R73C8H16OOH+O2=R136C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 51 CN
R74C8H16OOH+O2=R137C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 52 CN
R75C8H16OOH+O2=R139C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 53 CN
R76C8H16OOH+O2=R141C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 54 CN
R77C8H16OOH+O2=R142C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 55 CN
R78C8H16OOH+O2=R143C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 56 CN
R80C8H16OOH+O2=R145C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 57 CN
R81C8H16OOH+O2=R146C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 58 CN
R82C8H16OOH+O2=R147C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 59 CN
R83C8H16OOH+O2=R148C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 60 CN
R90C4H8OOH+O2=R165C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 61 CN
R94C7H14OOH+O2=R181C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 62 CN
R95C5H10OOH+O2=R182C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 63 CN
R98C5H10OOH+O2=R194C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 64 CN
R101C3H6OOH+O2=R200C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 65 CN
R103C7H14OOH+O2=R206C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 66 CN
R104C4H8OOH+O2=R156C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 67 CN
R106C5H10OOH+O2=R212C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 68 CN
R108C7H14OOH+O2=R219C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 69 CN
R112C7H14OOH+O2=R226C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 70 CN
R113C3H6OOH+O2=R152C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 71 CN
R115C4H8OOH+O2=R162C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 72 CN
R117C7H14OOH+O2=R234C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 73 CN
R118C7H14OOH+O2=R235C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 74 CN
R121C7H14OOH+O2=R242C7H14OOOOH    2.2E+19  -2.5  0.0  ! ADO 75 CN
R123C5H10OOH+O2=R246C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 76 CN
R124C5H10OOH+O2=R247C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 77 CN
R125C5H10OOH+O2=R248C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 78 CN
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R126C5H10OOH+O2=R249C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 79 CN
R131C8H16OOH+O2=R264C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 80 CN
R132C4H8OOH+O2=R265C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 81 CN
R134C5H10OOH+O2=R271C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 82 CN
R135C4H8OOH+O2=R272C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 83 CN
R138C5H10OOH+O2=R280C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 84 CN
R140C4H8OOH+O2=R282C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 85 CN
R144C4H8OOH+O2=R286C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 86 CN
R149C8H16OOH+O2=R294C8H16OOOOH    2.2E+19  -2.5  0.0  ! ADO 87 CN
R183C5H10OOH+O2=R310C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 88 CN
R184C5H10OOH+O2=R311C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 89 CN
R214C5H10OOH+O2=R334C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 90 CN
R250C5H10OOH+O2=R363C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 91 CN
R312C5H10OOH+O2=R388C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 92 CN
R327C4H8OOH+O2=R389C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 93 CN
R328C4H9+O2=R207C4H9OO    2.2E+19  -2.5  0.0  ! ADO 94 CN
R333C5H11+O2=R213C5H11OO    2.2E+19  -2.5  0.0  ! ADO 95 CN
R348C3H7+O2=R227C3H7OO    2.2E+19  -2.5  0.0  ! ADO 96 CN
R416C4H8OOH+O2=R411C4H8OOOOH    2.2E+19  -2.5  0.0  ! ADO 97 CN
R417C5H10OOH+O2=R412C5H10OOOOH    2.2E+19  -2.5  0.0  ! ADO 98 CN
R418C3H6OOH+O2=R414C3H6OOOOH    2.2E+19  -2.5  0.0  ! ADO 99 CN

!   isomerisations :
R21C7H15=R24C7H15    1.2E+12  0.0  19800.0  ! IS 100 KB
R22C7H15=R23C7H15    4.0E+11  0.0  17300.0  ! IS 101 KB
R22C7H15=R24C7H15    1.0E+11  0.0  14500.0  ! IS 102 KB
R23C7H15=R24C7H15    1.8E+10  0.0  19900.0  ! IS 103 KB
R25C8H17=R27C8H17    2.0E+11  0.0  15300.0  ! IS 104 KB
R25C8H17=R28C8H17    2.1E+11  0.0  14500.0  ! IS 105 KB
R29C3H7OO=R43C3H6OOH    2.3E+12  0.0  32500.0  ! IS 106 KB
R29C3H7OO=R44C3H6OOH    6.0E+11  0.0  28500.0  ! IS 107 KB
R30C4H9OO=R45C4H8OOH    2.3E+12  0.0  32500.0  ! IS 108 KB
R30C4H9OO=R46C4H8OOH    4.0E+11  0.0  25500.0  ! IS 109 KB
R30C4H9OO=R47C4H8OOH    1.0E+11  0.0  25000.0  ! IS 110 KB
R31C7H15OO=R48C7H14OOH    4.7E+12  0.0  32500.0  ! IS 111 KB
R31C7H15OO=R49C7H14OOH    8.0E+11  0.0  25500.0  ! IS 112 KB
R31C7H15OO=R50C7H14OOH    2.1E+11  0.0  25000.0  ! IS 113 KB
R32C7H15OO=R51C7H14OOH    2.3E+12  0.0  32500.0  ! IS 114 KB
R32C7H15OO=R52C7H14OOH    6.0E+11  0.0  28500.0  ! IS 115 KB
R32C7H15OO=R53C7H14OOH    2.3E+12  0.0  32500.0  ! IS 116 KB
R32C7H15OO=R54C7H14OOH    4.0E+11  0.0  25500.0  ! IS 117 KB
R32C7H15OO=R55C7H14OOH    6.9E+10  0.0  22000.0  ! IS 118 KB
R32C7H15OO=R56C7H14OOH    1.8E+10  0.0  24010.0  ! IS 119 KB
R33C7H15OO=R57C7H14OOH    3.5E+12  0.0  35500.0  ! IS 120 KB
R33C7H15OO=R58C7H14OOH    2.3E+12  0.0  32500.0  ! IS 121 KB
R33C7H15OO=R59C7H14OOH    4.0E+11  0.0  25500.0  ! IS 122 KB
R33C7H15OO=R60C7H14OOH    6.9E+10  0.0  22000.0  ! IS 123 KB
R33C7H15OO=R61C7H14OOH    1.2E+10  0.0  21010.0  ! IS 124 KB
R34C7H15OO=R62C7H14OOH    2.3E+12  0.0  32500.0  ! IS 125 KB
R34C7H15OO=R63C7H14OOH    4.0E+11  0.0  25500.0  ! IS 126 KB
R34C7H15OO=R64C7H14OOH    6.9E+10  0.0  22000.0  ! IS 127 KB
R34C7H15OO=R65C7H14OOH    1.2E+10  0.0  21010.0  ! IS 128 KB
R35C5H11=R67C5H11    4.0E+11  0.0  17300.0  ! IS 129 KB
R36C8H17OO=R68C8H16OOH    1.2E+12  0.0  28500.0  ! IS 130 KB
R36C8H17OO=R69C8H16OOH    4.0E+11  0.0  25500.0  ! IS 131 KB
R36C8H17OO=R70C8H16OOH    3.5E+10  0.0  19000.0  ! IS 132 KB
R36C8H17OO=R71C8H16OOH    3.6E+10  0.0  24010.0  ! IS 133 KB
R38C8H17OO=R73C8H16OOH    1.2E+12  0.0  29500.0  ! IS 134 KB
R38C8H17OO=R74C8H16OOH    1.2E+12  0.0  28500.0  ! IS 135 KB
R38C8H17OO=R75C8H16OOH    1.8E+12  0.0  28500.0  ! IS 136 KB
R39C8H17OO=R76C8H16OOH    7.0E+12  0.0  35500.0  ! IS 137 KB
R39C8H17OO=R77C8H16OOH    2.3E+12  0.0  32500.0  ! IS 138 KB
R39C8H17OO=R78C8H16OOH    3.1E+11  0.0  25000.0  ! IS 139 KB
R41C8H17OO=R80C8H16OOH    1.2E+12  0.0  29500.0  ! IS 140 KB
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R41C8H17OO=R81C8H16OOH    6.0E+11  0.0  28500.0  ! IS 141 KB
R41C8H17OO=R82C8H16OOH    4.0E+11  0.0  25500.0  ! IS 142 KB
R41C8H17OO=R83C8H16OOH    5.3E+10  0.0  24010.0  ! IS 143 KB
R47C4H8OOH=R90C4H8OOH    4.0E+11  0.0  17300.0  ! IS 144 KB
R48C7H14OOH=R49C7H14OOH    4.0E+11  0.0  17300.0  ! IS 145 KB
R48C7H14OOH=R50C7H14OOH    1.0E+11  0.0  14500.0  ! IS 146 KB
R49C7H14OOH=R50C7H14OOH    1.8E+10  0.0  19900.0  ! IS 147 KB
R50C7H14OOH=R94C7H14OOH    2.0E+11  0.0  15300.0  ! IS 148 KB
R51C7H14OOH=R54C7H14OOH    4.0E+11  0.0  17300.0  ! IS 149 KB
R51C7H14OOH=R55C7H14OOH    6.9E+10  0.0  12000.0  ! IS 150 KB
R51C7H14OOH=R56C7H14OOH    1.8E+10  0.0  19900.0  ! IS 151 KB
R52C7H14OOH=R53C7H14OOH    4.0E+11  0.0  17300.0  ! IS 152 KB
R52C7H14OOH=R54C7H14OOH    6.9E+10  0.0  12000.0  ! IS 153 KB
R52C7H14OOH=R55C7H14OOH    1.2E+10  0.0  17400.0  ! IS 154 KB
R52C7H14OOH=R56C7H14OOH    3.1E+09  0.0  23400.0  ! IS 155 KB
R53C7H14OOH=R56C7H14OOH    6.0E+11  0.0  19800.0  ! IS 156 KB
R55C7H14OOH=R103C7H14OOH    2.0E+11  0.0  15300.0  ! IS 157 KB
R56C7H14OOH=R103C7H14OOH    3.5E+10  0.0  10000.0  ! IS 158 KB
R57C7H14OOH=R59C7H14OOH    4.0E+11  0.0  17300.0  ! IS 159 KB
R57C7H14OOH=R60C7H14OOH    6.9E+10  0.0  12000.0  ! IS 160 KB
R57C7H14OOH=R61C7H14OOH    1.2E+10  0.0  17400.0  ! IS 161 KB
R57C7H14OOH=R108C7H14OOH    3.1E+09  0.0  23400.0  ! IS 162 KB
R58C7H14OOH=R61C7H14OOH    4.0E+11  0.0  17300.0  ! IS 163 KB
R58C7H14OOH=R108C7H14OOH    1.0E+11  0.0  14500.0  ! IS 164 KB
R59C7H14OOH=R108C7H14OOH    6.0E+11  0.0  19800.0  ! IS 165 KB
R60C7H14OOH=R112C7H14OOH    2.0E+11  0.0  15300.0  ! IS 166 KB
R61C7H14OOH=R112C7H14OOH    3.5E+10  0.0  10000.0  ! IS 167 KB
R62C7H14OOH=R65C7H14OOH    4.0E+11  0.0  17300.0  ! IS 168 KB
R62C7H14OOH=R117C7H14OOH    6.9E+10  0.0  12000.0  ! IS 169 KB
R62C7H14OOH=R118C7H14OOH    1.8E+10  0.0  19900.0  ! IS 170 KB
R63C7H14OOH=R117C7H14OOH    4.0E+11  0.0  17300.0  ! IS 171 KB
R63C7H14OOH=R118C7H14OOH    1.0E+11  0.0  14500.0  ! IS 172 KB
R64C7H14OOH=R118C7H14OOH    6.0E+11  0.0  19800.0  ! IS 173 KB
R64C7H14OOH=R121C7H14OOH    4.0E+11  0.0  17300.0  ! IS 174 KB
R65C7H14OOH=R121C7H14OOH    6.9E+10  0.0  12000.0  ! IS 175 KB
R66C5H11OO=R123C5H10OOH    2.3E+12  0.0  32500.0  ! IS 176 KB
R66C5H11OO=R124C5H10OOH    4.0E+11  0.0  25500.0  ! IS 177 KB
R66C5H11OO=R125C5H10OOH    6.9E+10  0.0  22000.0  ! IS 178 KB
R66C5H11OO=R126C5H10OOH    1.8E+10  0.0  24010.0  ! IS 179 KB
R68C8H16OOH=R70C8H16OOH    2.0E+11  0.0  15300.0  ! IS 180 KB
R68C8H16OOH=R71C8H16OOH    2.1E+11  0.0  14500.0  ! IS 181 KB
R70C8H16OOH=R131C8H16OOH    4.0E+11  0.0  17300.0  ! IS 182 KB
R71C8H16OOH=R131C8H16OOH    6.9E+10  0.0  12000.0  ! IS 183 KB
R72C4H9OO=R132C4H8OOH    1.2E+12  0.0  29500.0  ! IS 184 KB
R72C4H9OO=R135C4H8OOH    1.2E+12  0.0  28500.0  ! IS 185 KB
R73C8H16OOH=R75C8H16OOH    1.8E+12  0.0  19800.0  ! IS 186 KB
R74C8H16OOH=R75C8H16OOH    3.1E+11  0.0  14500.0  ! IS 187 KB
R76C8H16OOH=R78C8H16OOH    3.1E+11  0.0  14500.0  ! IS 188 KB
R79C4H9OO=R144C4H8OOH    1.1E+13  0.0  35500.0  ! IS 189 KB
R80C8H16OOH=R83C8H16OOH    1.8E+12  0.0  19800.0  ! IS 190 KB
R81C8H16OOH=R83C8H16OOH    3.1E+11  0.0  14500.0  ! IS 191 KB
R83C8H16OOH=R149C8H16OOH    6.9E+10  0.0  12000.0  ! IS 192 KB
R84C5H11OO=R134C5H10OOH    1.8E+12  0.0  28500.0  ! IS 193 KB
R85C3H6OOOOH=R150C3H5O4H2    3.5E+12  0.0  35500.0  ! IS 194 KB
R85C3H6OOOOH=R151C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 195 KB
R85C3H6OOOOH=R152C3H6OOOOH    3.5E+10  0.0  25000.0  ! IS 196 KB
R86C3H6OOOOH=R153C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 197 KB
R86C3H6OOOOH=R154C3H5O4H2    4.0E+11  0.0  25500.0  ! IS 198 KB
R87C4H8OOOOH=R155C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 199 KB
R87C4H8OOOOH=R156C4H8OOOOH    3.5E+10  0.0  25000.0  ! IS 200 KB
R87C4H8OOOOH=R157C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 201 KB
R87C4H8OOOOH=R158C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 202 KB
R88C4H8OOOOH=R159C4H7O4H2    3.5E+12  0.0  35500.0  ! IS 203 KB
R88C4H8OOOOH=R160C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 204 KB
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R88C4H8OOOOH=R161C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 205 KB
R88C4H8OOOOH=R162C4H8OOOOH    5.9E+09  0.0  24010.0  ! IS 206 KB
R89C4H8OOOOH=R163C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 207 KB
R89C4H8OOOOH=R164C4H7O4H2    6.9E+10  0.0  22000.0  ! IS 208 KB
R91C7H14OOOOH=R166C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 209 KB
R91C7H14OOOOH=R167C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 210 KB
R91C7H14OOOOH=R168C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 211 KB
R91C7H14OOOOH=R99C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 212 KB
R91C7H14OOOOH=R169C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 213 KB
R91C7H14OOOOH=R170C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 214 KB
R91C7H14OOOOH=R171C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 215 KB
R92C7H14OOOOH=R172C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 216 KB
R92C7H14OOOOH=R173C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 217 KB
R92C7H14OOOOH=R174C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 218 KB
R92C7H14OOOOH=R110C7H14OOOOH    5.9E+09  0.0  24010.0  ! IS 219 KB
R92C7H14OOOOH=R175C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 220 KB
R92C7H14OOOOH=R176C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 221 KB
R93C7H14OOOOH=R177C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 222 KB
R93C7H14OOOOH=R178C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 223 KB
R93C7H14OOOOH=R179C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 224 KB
R93C7H14OOOOH=R180C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 225 KB
R127C5H11OO=R95C5H10OOH    3.5E+12  0.0  35500.0  ! IS 226 KB
R95C5H10OOH=R183C5H10OOH    4.0E+11  0.0  17300.0  ! IS 227 KB
R95C5H10OOH=R184C5H10OOH    1.0E+11  0.0  14500.0  ! IS 228 KB
R96C7H14OOOOH=R185C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 229 KB
R96C7H14OOOOH=R186C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 230 KB
R96C7H14OOOOH=R109C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 231 KB
R96C7H14OOOOH=R187C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 232 KB
R96C7H14OOOOH=R188C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 233 KB
R96C7H14OOOOH=R189C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 234 KB
R97C7H14OOOOH=R190C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 235 KB
R97C7H14OOOOH=R191C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 236 KB
R97C7H14OOOOH=R119C7H14OOOOH    5.9E+09  0.0  24010.0  ! IS 237 KB
R97C7H14OOOOH=R192C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 238 KB
R97C7H14OOOOH=R193C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 239 KB
R98C5H10OOH=R125C5H10OOH    4.0E+11  0.0  17300.0  ! IS 240 KB
R98C5H10OOH=R126C5H10OOH    1.0E+11  0.0  14500.0  ! IS 241 KB
R99C7H14OOOOH=R169C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 242 KB
R99C7H14OOOOH=R170C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 243 KB
R99C7H14OOOOH=R171C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 244 KB
R99C7H14OOOOH=R195C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 245 KB
R99C7H14OOOOH=R166C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 246 KB
R99C7H14OOOOH=R167C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 247 KB
R100C7H14OOOOH=R196C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 248 KB
R100C7H14OOOOH=R197C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 249 KB
R100C7H14OOOOH=R198C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 250 KB
R100C7H14OOOOH=R199C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 251 KB
R102C7H14OOOOH=R201C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 252 KB
R102C7H14OOOOH=R202C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 253 KB
R102C7H14OOOOH=R203C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 254 KB
R102C7H14OOOOH=R204C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 255 KB
R102C7H14OOOOH=R205C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 256 KB
R207C4H9OO=R104C4H8OOH    3.5E+12  0.0  35500.0  ! IS 257 KB
R104C4H8OOH=R115C4H8OOH    6.0E+11  0.0  19800.0  ! IS 258 KB
R105C7H14OOOOH=R208C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 259 KB
R105C7H14OOOOH=R209C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 260 KB
R105C7H14OOOOH=R210C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 261 KB
R105C7H14OOOOH=R211C7H13O4H2    5.9E+09  0.0  16010.0  ! IS 262 KB
R213C5H11OO=R106C5H10OOH    1.2E+12  0.0  28500.0  ! IS 263 KB
R106C5H10OOH=R214C5H10OOH    4.0E+11  0.0  17300.0  ! IS 264 KB
R107C7H14OOOOH=R215C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 265 KB
R107C7H14OOOOH=R116C7H14OOOOH    3.5E+10  0.0  25000.0  ! IS 266 KB
R107C7H14OOOOH=R216C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 267 KB
R107C7H14OOOOH=R217C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 268 KB
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R107C7H14OOOOH=R218C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 269 KB
R108C7H14OOH=R112C7H14OOH    5.9E+09  0.0  15400.0  ! IS 270 KB
R109C7H14OOOOH=R220C7H13O4H2    1.2E+12  0.0  29500.0  ! IS 271 KB
R109C7H14OOOOH=R185C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 272 KB
R109C7H14OOOOH=R187C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 273 KB
R109C7H14OOOOH=R188C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 274 KB
R109C7H14OOOOH=R189C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 275 KB
R109C7H14OOOOH=R221C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 276 KB
R110C7H14OOOOH=R175C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 277 KB
R110C7H14OOOOH=R176C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 278 KB
R110C7H14OOOOH=R222C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 279 KB
R110C7H14OOOOH=R173C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 280 KB
R110C7H14OOOOH=R223C7H13O4H2    2.0E+11  0.0  22500.0  ! IS 281 KB
R110C7H14OOOOH=R172C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 282 KB
R111C7H14OOOOH=R205C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 283 KB
R111C7H14OOOOH=R224C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 284 KB
R111C7H14OOOOH=R203C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 285 KB
R111C7H14OOOOH=R202C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 286 KB
R111C7H14OOOOH=R225C7H13O4H2    3.5E+10  0.0  19000.0  ! IS 287 KB
R111C7H14OOOOH=R201C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 288 KB
R227C3H7OO=R113C3H6OOH    7.0E+12  0.0  35500.0  ! IS 289 KB
R114C7H14OOOOH=R228C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 290 KB
R114C7H14OOOOH=R229C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 291 KB
R114C7H14OOOOH=R230C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 292 KB
R114C7H14OOOOH=R231C7H13O4H2    5.9E+09  0.0  16010.0  ! IS 293 KB
R207C4H9OO=R115C4H8OOH    6.0E+11  0.0  28500.0  ! IS 294 KB
R116C7H14OOOOH=R232C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 295 KB
R116C7H14OOOOH=R216C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 296 KB
R116C7H14OOOOH=R217C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 297 KB
R116C7H14OOOOH=R218C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 298 KB
R116C7H14OOOOH=R233C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 299 KB
R117C7H14OOH=R121C7H14OOH    1.2E+10  0.0  17400.0  ! IS 300 KB
R118C7H14OOH=R121C7H14OOH    2.0E+09  0.0  20900.0  ! IS 301 KB
R119C7H14OOOOH=R190C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 302 KB
R119C7H14OOOOH=R236C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 303 KB
R119C7H14OOOOH=R192C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 304 KB
R119C7H14OOOOH=R193C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 305 KB
R119C7H14OOOOH=R237C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 306 KB
R119C7H14OOOOH=R238C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 307 KB
R120C7H14OOOOH=R180C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 308 KB
R120C7H14OOOOH=R239C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 309 KB
R120C7H14OOOOH=R240C7H13O4H2    1.0E+11  0.0  25000.0  ! IS 310 KB
R120C7H14OOOOH=R178C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 311 KB
R120C7H14OOOOH=R177C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 312 KB
R120C7H14OOOOH=R241C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 313 KB
R122C7H14OOOOH=R243C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 314 KB
R122C7H14OOOOH=R244C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 315 KB
R122C7H14OOOOH=R210C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 316 KB
R122C7H14OOOOH=R209C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 317 KB
R122C7H14OOOOH=R208C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 318 KB
R122C7H14OOOOH=R245C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 319 KB
R123C5H10OOH=R126C5H10OOH    6.0E+11  0.0  19800.0  ! IS 320 KB
R127C5H11OO=R250C5H10OOH    2.3E+12  0.0  32500.0  ! IS 321 KB
R127C5H11OO=R183C5H10OOH    4.0E+11  0.0  25500.0  ! IS 322 KB
R127C5H11OO=R184C5H10OOH    1.0E+11  0.0  25000.0  ! IS 323 KB
R128C8H16OOOOH=R251C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 324 KB
R128C8H16OOOOH=R252C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 325 KB
R128C8H16OOOOH=R253C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 326 KB
R128C8H16OOOOH=R254C8H15O4H2    3.5E+10  0.0  19000.0  ! IS 327 KB
R128C8H16OOOOH=R255C8H15O4H2    3.6E+10  0.0  24010.0  ! IS 328 KB
R129C8H16OOOOH=R256C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 329 KB
R129C8H16OOOOH=R257C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 330 KB
R129C8H16OOOOH=R258C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 331 KB
R129C8H16OOOOH=R259C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 332 KB
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R129C8H16OOOOH=R139C8H16OOOOH    5.9E+09  0.0  24010.0  ! IS 333 KB
R130C8H16OOOOH=R260C8H15O4H2    7.0E+12  0.0  35500.0  ! IS 334 KB
R130C8H16OOOOH=R261C8H15O4H2    2.3E+12  0.0  32500.0  ! IS 335 KB
R130C8H16OOOOH=R262C8H15O4H2    2.1E+11  0.0  25000.0  ! IS 336 KB
R130C8H16OOOOH=R263C8H15O4H2    6.9E+10  0.0  22000.0  ! IS 337 KB
R133C8H16OOOOH=R266C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 338 KB
R133C8H16OOOOH=R267C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 339 KB
R133C8H16OOOOH=R268C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 340 KB
R133C8H16OOOOH=R269C8H15O4H2    3.6E+10  0.0  24010.0  ! IS 341 KB
R133C8H16OOOOH=R270C8H15O4H2    1.2E+10  0.0  21010.0  ! IS 342 KB
R136C8H16OOOOH=R273C8H15O4H2    7.0E+12  0.0  35500.0  ! IS 343 KB
R136C8H16OOOOH=R274C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 344 KB
R136C8H16OOOOH=R142C8H16OOOOH    3.5E+10  0.0  25000.0  ! IS 345 KB
R136C8H16OOOOH=R275C8H15O4H2    3.1E+11  0.0  25000.0  ! IS 346 KB
R137C8H16OOOOH=R276C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 347 KB
R137C8H16OOOOH=R277C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 348 KB
R137C8H16OOOOH=R278C8H15O4H2    2.0E+11  0.0  22500.0  ! IS 349 KB
R137C8H16OOOOH=R147C8H16OOOOH    5.9E+09  0.0  24010.0  ! IS 350 KB
R137C8H16OOOOH=R279C8H15O4H2    5.3E+10  0.0  24010.0  ! IS 351 KB
R139C8H16OOOOH=R258C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 352 KB
R139C8H16OOOOH=R281C8H15O4H2    2.0E+11  0.0  22500.0  ! IS 353 KB
R139C8H16OOOOH=R256C8H15O4H2    3.5E+10  0.0  19000.0  ! IS 354 KB
R139C8H16OOOOH=R257C8H15O4H2    3.6E+10  0.0  24010.0  ! IS 355 KB
R141C8H16OOOOH=R145C8H16OOOOH    3.5E+10  0.0  25000.0  ! IS 356 KB
R141C8H16OOOOH=R283C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 357 KB
R141C8H16OOOOH=R284C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 358 KB
R141C8H16OOOOH=R285C8H15O4H2    5.3E+10  0.0  24010.0  ! IS 359 KB
R142C8H16OOOOH=R273C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 360 KB
R142C8H16OOOOH=R275C8H15O4H2    1.8E+12  0.0  28500.0  ! IS 361 KB
R143C8H16OOOOH=R262C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 362 KB
R143C8H16OOOOH=R261C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 363 KB
R143C8H16OOOOH=R260C8H15O4H2    3.6E+10  0.0  24010.0  ! IS 364 KB
R145C8H16OOOOH=R283C8H15O4H2    3.5E+12  0.0  35500.0  ! IS 365 KB
R145C8H16OOOOH=R287C8H15O4H2    2.3E+12  0.0  32500.0  ! IS 366 KB
R145C8H16OOOOH=R284C8H15O4H2    2.3E+12  0.0  32500.0  ! IS 367 KB
R145C8H16OOOOH=R285C8H15O4H2    3.1E+11  0.0  25000.0  ! IS 368 KB
R146C8H16OOOOH=R288C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 369 KB
R146C8H16OOOOH=R289C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 370 KB
R146C8H16OOOOH=R290C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 371 KB
R146C8H16OOOOH=R291C8H15O4H2    5.3E+10  0.0  24010.0  ! IS 372 KB
R147C8H16OOOOH=R279C8H15O4H2    1.8E+12  0.0  28500.0  ! IS 373 KB
R147C8H16OOOOH=R276C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 374 KB
R147C8H16OOOOH=R277C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 375 KB
R147C8H16OOOOH=R292C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 376 KB
R148C8H16OOOOH=R269C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 377 KB
R148C8H16OOOOH=R268C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 378 KB
R148C8H16OOOOH=R266C8H15O4H2    3.5E+10  0.0  19000.0  ! IS 379 KB
R148C8H16OOOOH=R267C8H15O4H2    1.8E+10  0.0  24010.0  ! IS 380 KB
R148C8H16OOOOH=R293C8H15O4H2    1.2E+10  0.0  21010.0  ! IS 381 KB
R152C3H6OOOOH=R150C3H5O4H2    6.0E+11  0.0  28500.0  ! IS 382 KB
R152C3H6OOOOH=R295C3H5O4H2    1.2E+12  0.0  29500.0  ! IS 383 KB
R155C4H7O4H2=R158C4H7O4H2    6.0E+11  0.0  19800.0  ! IS 384 KB
R156C4H8OOOOH=R296C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 385 KB
R156C4H8OOOOH=R157C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 386 KB
R156C4H8OOOOH=R158C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 387 KB
R159C4H7O4H2=R161C4H7O4H2    4.0E+11  0.0  17300.0  ! IS 388 KB
R162C4H8OOOOH=R159C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 389 KB
R162C4H8OOOOH=R160C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 390 KB
R162C4H8OOOOH=R297C4H7O4H2    2.0E+11  0.0  22500.0  ! IS 391 KB
R165C4H8OOOOH=R298C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 392 KB
R165C4H8OOOOH=R299C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 393 KB
R165C4H8OOOOH=R300C4H7O4H2    1.0E+11  0.0  25000.0  ! IS 394 KB
R166C7H13O4H2=R169C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 395 KB
R166C7H13O4H2=R170C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 396 KB
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R166C7H13O4H2=R171C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 397 KB
R167C7H13O4H2=R168C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 398 KB
R167C7H13O4H2=R169C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 399 KB
R167C7H13O4H2=R170C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 400 KB
R167C7H13O4H2=R171C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 401 KB
R168C7H13O4H2=R171C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 402 KB
R170C7H13O4H2=R195C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 403 KB
R171C7H13O4H2=R195C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 404 KB
R172C7H13O4H2=R174C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 405 KB
R172C7H13O4H2=R175C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 406 KB
R172C7H13O4H2=R176C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 407 KB
R172C7H13O4H2=R222C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 408 KB
R173C7H13O4H2=R176C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 409 KB
R173C7H13O4H2=R222C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 410 KB
R174C7H13O4H2=R222C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 411 KB
R175C7H13O4H2=R223C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 412 KB
R176C7H13O4H2=R223C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 413 KB
R177C7H13O4H2=R180C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 414 KB
R177C7H13O4H2=R239C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 415 KB
R177C7H13O4H2=R240C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 416 KB
R178C7H13O4H2=R239C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 417 KB
R178C7H13O4H2=R240C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 418 KB
R179C7H13O4H2=R240C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 419 KB
R179C7H13O4H2=R241C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 420 KB
R180C7H13O4H2=R241C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 421 KB
R181C7H14OOOOH=R303C7H13O4H2    4.7E+12  0.0  32500.0  ! IS 422 KB
R181C7H14OOOOH=R304C7H13O4H2    8.0E+11  0.0  25500.0  ! IS 423 KB
R181C7H14OOOOH=R305C7H13O4H2    2.1E+11  0.0  25000.0  ! IS 424 KB
R182C5H10OOOOH=R306C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 425 KB
R182C5H10OOOOH=R246C5H10OOOOH    3.5E+10  0.0  25000.0  ! IS 426 KB
R182C5H10OOOOH=R307C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 427 KB
R182C5H10OOOOH=R308C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 428 KB
R182C5H10OOOOH=R309C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 429 KB
R184C5H10OOH=R312C5H10OOH    2.0E+11  0.0  15300.0  ! IS 430 KB
R185C7H13O4H2=R187C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 431 KB
R185C7H13O4H2=R188C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 432 KB
R185C7H13O4H2=R189C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 433 KB
R185C7H13O4H2=R221C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 434 KB
R186C7H13O4H2=R189C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 435 KB
R186C7H13O4H2=R221C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 436 KB
R187C7H13O4H2=R221C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 437 KB
R188C7H13O4H2=R220C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 438 KB
R189C7H13O4H2=R220C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 439 KB
R190C7H13O4H2=R193C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 440 KB
R190C7H13O4H2=R237C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 441 KB
R190C7H13O4H2=R238C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 442 KB
R191C7H13O4H2=R237C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 443 KB
R191C7H13O4H2=R238C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 444 KB
R192C7H13O4H2=R238C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 445 KB
R192C7H13O4H2=R236C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 446 KB
R193C7H13O4H2=R236C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 447 KB
R194C5H10OOOOH=R314C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 448 KB
R194C5H10OOOOH=R315C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 449 KB
R194C5H10OOOOH=R316C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 450 KB
R194C5H10OOOOH=R317C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 451 KB
R196C7H13O4H2=R199C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 452 KB
R196C7H13O4H2=R197C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 453 KB
R197C7H13O4H2=R198C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 454 KB
R197C7H13O4H2=R199C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 455 KB
R200C3H6OOOOH=R319C3H5O4H2    2.3E+12  0.0  32500.0  ! IS 456 KB
R200C3H6OOOOH=R320C3H5O4H2    6.0E+11  0.0  28500.0  ! IS 457 KB
R201C7H13O4H2=R203C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 458 KB
R201C7H13O4H2=R204C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 459 KB
R201C7H13O4H2=R205C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 460 KB
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R201C7H13O4H2=R224C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 461 KB
R202C7H13O4H2=R205C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 462 KB
R202C7H13O4H2=R224C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 463 KB
R203C7H13O4H2=R224C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 464 KB
R204C7H13O4H2=R225C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 465 KB
R205C7H13O4H2=R225C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 466 KB
R206C7H14OOOOH=R321C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 467 KB
R206C7H14OOOOH=R322C7H13O4H2    6.0E+11  0.0  28500.0  ! IS 468 KB
R206C7H14OOOOH=R323C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 469 KB
R206C7H14OOOOH=R324C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 470 KB
R206C7H14OOOOH=R325C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 471 KB
R206C7H14OOOOH=R326C7H13O4H2    1.8E+10  0.0  24010.0  ! IS 472 KB
R207C4H9OO=R327C4H8OOH    2.3E+12  0.0  32500.0  ! IS 473 KB
R208C7H13O4H2=R211C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 474 KB
R208C7H13O4H2=R243C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 475 KB
R208C7H13O4H2=R244C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 476 KB
R209C7H13O4H2=R243C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 477 KB
R209C7H13O4H2=R244C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 478 KB
R210C7H13O4H2=R244C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 479 KB
R210C7H13O4H2=R245C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 480 KB
R211C7H13O4H2=R245C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 481 KB
R212C5H10OOOOH=R329C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 482 KB
R212C5H10OOOOH=R330C5H9O4H2    2.0E+11  0.0  22500.0  ! IS 483 KB
R212C5H10OOOOH=R247C5H10OOOOH    5.9E+09  0.0  24010.0  ! IS 484 KB
R212C5H10OOOOH=R331C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 485 KB
R212C5H10OOOOH=R332C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 486 KB
R213C5H11OO=R214C5H10OOH    4.7E+12  0.0  32500.0  ! IS 487 KB
R215C7H13O4H2=R218C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 488 KB
R215C7H13O4H2=R233C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 489 KB
R215C7H13O4H2=R335C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 490 KB
R216C7H13O4H2=R233C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 491 KB
R216C7H13O4H2=R335C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 492 KB
R217C7H13O4H2=R335C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 493 KB
R217C7H13O4H2=R232C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 494 KB
R218C7H13O4H2=R232C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 495 KB
R219C7H14OOOOH=R336C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 496 KB
R219C7H14OOOOH=R337C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 497 KB
R219C7H14OOOOH=R338C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 498 KB
R219C7H14OOOOH=R339C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 499 KB
R220C7H13O4H2=R221C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 500 KB
R222C7H13O4H2=R223C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 501 KB
R224C7H13O4H2=R225C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 502 KB
R226C7H14OOOOH=R343C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 503 KB
R226C7H14OOOOH=R344C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 504 KB
R226C7H14OOOOH=R345C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 505 KB
R226C7H14OOOOH=R346C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 506 KB
R226C7H14OOOOH=R347C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 507 KB
R228C7H13O4H2=R230C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 508 KB
R228C7H13O4H2=R229C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 509 KB
R228C7H13O4H2=R231C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 510 KB
R229C7H13O4H2=R231C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 511 KB
R232C7H13O4H2=R233C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 512 KB
R232C7H13O4H2=R335C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 513 KB
R234C7H14OOOOH=R349C7H13O4H2    3.5E+12  0.0  35500.0  ! IS 514 KB
R234C7H14OOOOH=R339C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 515 KB
R234C7H14OOOOH=R338C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 516 KB
R234C7H14OOOOH=R337C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 517 KB
R234C7H14OOOOH=R336C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 518 KB
R235C7H14OOOOH=R350C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 519 KB
R235C7H14OOOOH=R351C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 520 KB
R235C7H14OOOOH=R352C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 521 KB
R236C7H13O4H2=R237C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 522 KB
R236C7H13O4H2=R238C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 523 KB
R239C7H13O4H2=R241C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 524 KB
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R240C7H13O4H2=R241C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 525 KB
R242C7H14OOOOH=R354C7H13O4H2    2.3E+12  0.0  32500.0  ! IS 526 KB
R242C7H14OOOOH=R355C7H13O4H2    4.0E+11  0.0  25500.0  ! IS 527 KB
R242C7H14OOOOH=R356C7H13O4H2    6.9E+10  0.0  22000.0  ! IS 528 KB
R242C7H14OOOOH=R357C7H13O4H2    1.2E+10  0.0  21010.0  ! IS 529 KB
R243C7H13O4H2=R245C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 530 KB
R244C7H13O4H2=R245C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 531 KB
R246C5H10OOOOH=R301C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 532 KB
R246C5H10OOOOH=R307C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 533 KB
R246C5H10OOOOH=R308C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 534 KB
R246C5H10OOOOH=R309C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 535 KB
R247C5H10OOOOH=R331C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 536 KB
R247C5H10OOOOH=R332C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 537 KB
R247C5H10OOOOH=R329C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 538 KB
R247C5H10OOOOH=R318C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 539 KB
R248C5H10OOOOH=R353C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 540 KB
R248C5H10OOOOH=R359C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 541 KB
R248C5H10OOOOH=R360C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 542 KB
R248C5H10OOOOH=R342C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 543 KB
R249C5H10OOOOH=R361C5H9O4H2    6.9E+10  0.0  22000.0  ! IS 544 KB
R249C5H10OOOOH=R362C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 545 KB
R249C5H10OOOOH=R358C5H9O4H2    1.2E+10  0.0  21010.0  ! IS 546 KB
R251C8H15O4H2=R254C8H15O4H2    2.0E+11  0.0  15300.0  ! IS 547 KB
R251C8H15O4H2=R255C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 548 KB
R252C8H15O4H2=R254C8H15O4H2    2.0E+11  0.0  15300.0  ! IS 549 KB
R252C8H15O4H2=R255C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 550 KB
R256C8H15O4H2=R258C8H15O4H2    1.2E+12  0.0  19800.0  ! IS 551 KB
R256C8H15O4H2=R259C8H15O4H2    4.0E+11  0.0  17300.0  ! IS 552 KB
R257C8H15O4H2=R258C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 553 KB
R257C8H15O4H2=R259C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 554 KB
R260C8H15O4H2=R262C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 555 KB
R260C8H15O4H2=R263C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 556 KB
R264C8H16OOOOH=R367C8H15O4H2    1.2E+12  0.0  28500.0  ! IS 557 KB
R264C8H16OOOOH=R368C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 558 KB
R264C8H16OOOOH=R369C8H15O4H2    3.5E+10  0.0  19000.0  ! IS 559 KB
R264C8H16OOOOH=R370C8H15O4H2    3.6E+10  0.0  24010.0  ! IS 560 KB
R265C4H8OOOOH=R371C4H7O4H2    7.0E+12  0.0  35500.0  ! IS 561 KB
R265C4H8OOOOH=R372C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 562 KB
R265C4H8OOOOH=R286C4H8OOOOH    3.5E+10  0.0  25000.0  ! IS 563 KB
R266C8H15O4H2=R269C8H15O4H2    1.2E+12  0.0  19800.0  ! IS 564 KB
R266C8H15O4H2=R270C8H15O4H2    4.0E+11  0.0  17300.0  ! IS 565 KB
R267C8H15O4H2=R269C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 566 KB
R267C8H15O4H2=R270C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 567 KB
R269C8H15O4H2=R293C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 568 KB
R270C8H15O4H2=R293C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 569 KB
R271C5H10OOOOH=R365C5H9O4H2    1.2E+12  0.0  28500.0  ! IS 570 KB
R271C5H10OOOOH=R366C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 571 KB
R272C4H8OOOOH=R364C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 572 KB
R272C4H8OOOOH=R373C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 573 KB
R272C4H8OOOOH=R374C4H7O4H2    4.0E+11  0.0  25500.0  ! IS 574 KB
R273C8H15O4H2=R275C8H15O4H2    3.1E+11  0.0  14500.0  ! IS 575 KB
R276C8H15O4H2=R279C8H15O4H2    1.8E+12  0.0  19800.0  ! IS 576 KB
R277C8H15O4H2=R279C8H15O4H2    3.1E+11  0.0  14500.0  ! IS 577 KB
R279C8H15O4H2=R292C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 578 KB
R280C5H10OOOOH=R375C5H9O4H2    1.8E+12  0.0  28500.0  ! IS 579 KB
R282C4H8OOOOH=R376C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 580 KB
R282C4H8OOOOH=R377C4H7O4H2    1.2E+12  0.0  28500.0  ! IS 581 KB
R283C8H15O4H2=R285C8H15O4H2    3.1E+11  0.0  14500.0  ! IS 582 KB
R285C8H15O4H2=R287C8H15O4H2    6.9E+10  0.0  12000.0  ! IS 583 KB
R286C4H8OOOOH=R371C4H7O4H2    1.2E+12  0.0  28500.0  ! IS 584 KB
R288C8H15O4H2=R291C8H15O4H2    1.8E+12  0.0  19800.0  ! IS 585 KB
R289C8H15O4H2=R291C8H15O4H2    3.1E+11  0.0  14500.0  ! IS 586 KB
R294C8H16OOOOH=R378C8H15O4H2    1.2E+12  0.0  29500.0  ! IS 587 KB
R294C8H16OOOOH=R379C8H15O4H2    6.0E+11  0.0  28500.0  ! IS 588 KB
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R294C8H16OOOOH=R380C8H15O4H2    4.0E+11  0.0  25500.0  ! IS 589 KB
R294C8H16OOOOH=R381C8H15O4H2    5.3E+10  0.0  24010.0  ! IS 590 KB
R300C4H7O4H2=R382C4H7O4H2    2.0E+11  0.0  15300.0  ! IS 591 KB
R301C5H9O4H2=R308C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 592 KB
R301C5H9O4H2=R309C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 593 KB
R334C5H10OOOOH=R302C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 594 KB
R363C5H10OOOOH=R302C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 595 KB
R302C5H9O4H2=R383C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 596 KB
R302C5H9O4H2=R340C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 597 KB
R303C7H13O4H2=R304C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 598 KB
R303C7H13O4H2=R305C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 599 KB
R304C7H13O4H2=R305C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 600 KB
R306C5H9O4H2=R309C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 601 KB
R310C5H10OOOOH=R341C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 602 KB
R310C5H10OOOOH=R385C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 603 KB
R310C5H10OOOOH=R386C5H9O4H2    2.0E+11  0.0  22500.0  ! IS 604 KB
R311C5H10OOOOH=R360C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 605 KB
R311C5H10OOOOH=R359C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 606 KB
R311C5H10OOOOH=R387C5H9O4H2    3.5E+10  0.0  19000.0  ! IS 607 KB
R311C5H10OOOOH=R353C5H9O4H2    1.8E+10  0.0  24010.0  ! IS 608 KB
R389C4H8OOOOH=R313C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 609 KB
R314C5H9O4H2=R317C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 610 KB
R316C5H9O4H2=R390C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 611 KB
R317C5H9O4H2=R390C5H9O4H2    3.5E+10  0.0  10000.0  ! IS 612 KB
R318C5H9O4H2=R331C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 613 KB
R318C5H9O4H2=R332C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 614 KB
R321C7H13O4H2=R324C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 615 KB
R321C7H13O4H2=R325C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 616 KB
R321C7H13O4H2=R326C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 617 KB
R322C7H13O4H2=R323C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 618 KB
R322C7H13O4H2=R324C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 619 KB
R322C7H13O4H2=R325C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 620 KB
R322C7H13O4H2=R326C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 621 KB
R323C7H13O4H2=R326C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 622 KB
R329C5H9O4H2=R332C5H9O4H2    6.0E+11  0.0  19800.0  ! IS 623 KB
R334C5H10OOOOH=R394C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 624 KB
R334C5H10OOOOH=R363C5H10OOOOH    3.5E+10  0.0  25000.0  ! IS 625 KB
R334C5H10OOOOH=R383C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 626 KB
R334C5H10OOOOH=R340C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 627 KB
R336C7H13O4H2=R339C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 628 KB
R336C7H13O4H2=R395C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 629 KB
R336C7H13O4H2=R349C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 630 KB
R337C7H13O4H2=R395C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 631 KB
R337C7H13O4H2=R349C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 632 KB
R338C7H13O4H2=R349C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 633 KB
R338C7H13O4H2=R396C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 634 KB
R339C7H13O4H2=R396C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 635 KB
R363C5H10OOOOH=R340C5H9O4H2    6.0E+11  0.0  28500.0  ! IS 636 KB
R340C5H9O4H2=R397C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 637 KB
R341C5H9O4H2=R386C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 638 KB
R342C5H9O4H2=R387C5H9O4H2    2.0E+11  0.0  15300.0  ! IS 639 KB
R342C5H9O4H2=R353C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 640 KB
R343C7H13O4H2=R345C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 641 KB
R343C7H13O4H2=R346C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 642 KB
R343C7H13O4H2=R347C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 643 KB
R343C7H13O4H2=R398C7H13O4H2    3.1E+09  0.0  23400.0  ! IS 644 KB
R344C7H13O4H2=R347C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 645 KB
R344C7H13O4H2=R398C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 646 KB
R345C7H13O4H2=R398C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 647 KB
R349C7H13O4H2=R396C7H13O4H2    2.0E+09  0.0  20900.0  ! IS 648 KB
R350C7H13O4H2=R351C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 649 KB
R350C7H13O4H2=R401C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 650 KB
R351C7H13O4H2=R401C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 651 KB
R352C7H13O4H2=R401C7H13O4H2    8.0E+11  0.0  17300.0  ! IS 652 KB
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R353C5H9O4H2=R360C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 653 KB
R354C7H13O4H2=R357C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 654 KB
R354C7H13O4H2=R402C7H13O4H2    6.9E+10  0.0  12000.0  ! IS 655 KB
R354C7H13O4H2=R403C7H13O4H2    1.8E+10  0.0  19900.0  ! IS 656 KB
R355C7H13O4H2=R402C7H13O4H2    4.0E+11  0.0  17300.0  ! IS 657 KB
R355C7H13O4H2=R403C7H13O4H2    1.0E+11  0.0  14500.0  ! IS 658 KB
R356C7H13O4H2=R403C7H13O4H2    6.0E+11  0.0  19800.0  ! IS 659 KB
R356C7H13O4H2=R404C7H13O4H2    2.0E+11  0.0  15300.0  ! IS 660 KB
R357C7H13O4H2=R404C7H13O4H2    3.5E+10  0.0  10000.0  ! IS 661 KB
R358C5H9O4H2=R361C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 662 KB
R363C5H10OOOOH=R383C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 663 KB
R363C5H10OOOOH=R397C5H9O4H2    1.2E+12  0.0  29500.0  ! IS 664 KB
R367C8H15O4H2=R369C8H15O4H2    2.0E+11  0.0  15300.0  ! IS 665 KB
R367C8H15O4H2=R370C8H15O4H2    2.1E+11  0.0  14500.0  ! IS 666 KB
R369C8H15O4H2=R405C8H15O4H2    2.0E+11  0.0  15300.0  ! IS 667 KB
R370C8H15O4H2=R405C8H15O4H2    3.5E+10  0.0  10000.0  ! IS 668 KB
R378C8H15O4H2=R381C8H15O4H2    1.8E+12  0.0  19800.0  ! IS 669 KB
R379C8H15O4H2=R381C8H15O4H2    3.1E+11  0.0  14500.0  ! IS 670 KB
R381C8H15O4H2=R406C8H15O4H2    3.5E+10  0.0  10000.0  ! IS 671 KB
R388C5H10OOOOH=R384C5H9O4H2    3.5E+12  0.0  35500.0  ! IS 672 KB
R384C5H9O4H2=R407C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 673 KB
R384C5H9O4H2=R408C5H9O4H2    1.0E+11  0.0  14500.0  ! IS 674 KB
R388C5H10OOOOH=R409C5H9O4H2    2.3E+12  0.0  32500.0  ! IS 675 KB
R388C5H10OOOOH=R407C5H9O4H2    4.0E+11  0.0  25500.0  ! IS 676 KB
R388C5H10OOOOH=R408C5H9O4H2    1.0E+11  0.0  25000.0  ! IS 677 KB
R389C4H8OOOOH=R410C4H7O4H2    1.2E+12  0.0  29500.0  ! IS 678 KB
R411C4H8OOOOH=R392C4H7O4H2    3.5E+12  0.0  35500.0  ! IS 679 KB
R392C4H7O4H2=R400C4H7O4H2    6.0E+11  0.0  19800.0  ! IS 680 KB
R412C5H10OOOOH=R393C5H9O4H2    1.2E+12  0.0  28500.0  ! IS 681 KB
R393C5H9O4H2=R413C5H9O4H2    4.0E+11  0.0  17300.0  ! IS 682 KB
R395C7H13O4H2=R396C7H13O4H2    1.2E+10  0.0  17400.0  ! IS 683 KB
R414C3H6OOOOH=R399C3H5O4H2    7.0E+12  0.0  35500.0  ! IS 684 KB
R411C4H8OOOOH=R400C4H7O4H2    6.0E+11  0.0  28500.0  ! IS 685 KB
R402C7H13O4H2=R404C7H13O4H2    5.9E+09  0.0  15400.0  ! IS 686 KB
R403C7H13O4H2=R404C7H13O4H2    1.0E+09  0.0  18900.0  ! IS 687 KB
R411C4H8OOOOH=R415C4H7O4H2    2.3E+12  0.0  32500.0  ! IS 688 KB
R412C5H10OOOOH=R413C5H9O4H2    4.7E+12  0.0  32500.0  ! IS 689 KB

!   beta-scissions :
R19C3H7=>R4CH3+C2H4Z    2.0E+13  0.0  31000.0  ! DE 690 CN
R20C4H9=>R11C2H5+C2H4Z    2.0E+13  0.0  28700.0  ! DE 691 CW
R21C7H15=>R11C2H5+C5H10Y    4.0E+13  0.0  28700.0  ! DE 692 CW
R22C7H15=>R19C3H7+C4H8Y    2.0E+13  0.0  28700.0  ! DE 693 CW
R22C7H15=>R4CH3+C6H12Z    2.0E+13  0.0  31000.0  ! DE 694 CN
R23C7H15=>R20C4H9+C3H6Y    2.0E+13  0.0  28700.0  ! DE 695 CW
R24C7H15=>R35C5H11+C2H4Z    2.0E+13  0.0  28700.0  ! DE 696 CW
R25C8H17=>R37C4H9+C4H8Y    2.0E+13  0.0  28700.0  ! DE 697 CW
R25C8H17=>R4CH3+C7H14Y    4.0E+13  0.0  31000.0  ! DE 698 CN
R26C8H17=>R4CH3+C7H14Y    4.0E+13  0.0  31000.0  ! DE 699 CN
     DUPLICATE
R26C8H17=>R4CH3+C7H14Y    6.0E+13  0.0  31000.0  ! DE 700 CN
     DUPLICATE
!R27C8H17=>R40C4H9+C4H8Y    2.0E+13  0.0  28700.0  ! DE 701 CW
R27C8H17=>R40C4H9+C4H8Y    2.0E+13  0.0  26700.0  ! DE 701 CW
R28C8H17=>R42C5H11+C3H6Y    2.0E+13  0.0  28700.0  ! DE 702 CW
R28C8H17=>R4CH3+C7H14Y    2.0E+13  0.0  31000.0  ! DE 703 CN
R35C5H11=>R19C3H7+C2H4Z    2.0E+13  0.0  28700.0  ! DE 704 CW
R37C4H9=>R4CH3+C3H6Y    4.0E+13  0.0  31000.0  ! DE 705 CN
R42C5H11=>R4CH3+C4H8Y    6.0E+13  0.0  31000.0  ! DE 706 CN
R43C3H6OOH=>R3O2H+C3H6Y    8.5E+12  0.0  26000.0  ! DE 707 CR
R45C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 708 CR
R45C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 709 CN
R47C4H8OOH=>R16C2H4O2H+C2H4Z    2.0E+13  0.0  28700.0  ! DE 710 CW
R48C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 711 CR
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R48C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 712 CN
R48C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 713 CW
R49C7H14OOH=>R90C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 714 CW
R50C7H14OOH=>R95C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 715 CW
R51C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 716 CR
R51C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 717 CW
R52C7H14OOH=>R98C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 718 CW
R53C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 719 CR
R53C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 720 CW
     DUPLICATE
R53C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 721 CW
     DUPLICATE
R54C7H14OOH=>R101C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 722 CW
R54C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 723 CN
R55C7H14OOH=>R104C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 724 CW
R56C7H14OOH=>R106C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 725 CW
R57C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 726 CR
R58C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 727 CR
R58C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 728 CN
R58C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 729 CW
R59C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 730 CW
R60C7H14OOH=>R113C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 731 CW
R60C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 732 CN
R61C7H14OOH=>R115C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 733 CW
R62C7H14OOH=>R3O2H+C7H14Y    8.5E+12  0.0  26000.0  ! DE 734 CR
R62C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 735 CW
R63C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 736 CW
R64C7H14OOH=>R16C2H4O2H+C5H10Y    2.0E+13  0.0  28700.0  ! DE 737 CW
R64C7H14OOH=>R11C2H5+C5H9OOHZ    2.0E+13  0.0  28700.0  ! DE 738 CW
R65C7H14OOH=>R44C3H6OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 739 CW
R65C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 740 CN
R67C5H11=>R11C2H5+C3H6Y    2.0E+13  0.0  28700.0  ! DE 741 CW
R68C8H16OOH=>R37C4H9+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 742 CW
R68C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 743 CN
R69C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 744 CN
     DUPLICATE
R69C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 745 CN
     DUPLICATE
R70C8H16OOH=>R132C4H8OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 746 CW
R71C8H16OOH=>R134C5H10OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 747 CW
R71C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 748 CN
R73C8H16OOH=>R3O2H+C8H16Y    8.5E+12  0.0  26000.0  ! DE 749 CR
R73C8H16OOH=>R40C4H9+C4H7OOHY    2.0E+13  0.0  26700.0  ! DE 750 CW
R74C8H16OOH=>R138C5H10OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 751 CW
R74C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 752 CN
R75C8H16OOH=>R140C4H8OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 753 CW
R75C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 754 CN
R76C8H16OOH=>R3O2H+C8H16Y    8.5E+12  0.0  26000.0  ! DE 755 CR
R76C8H16OOH=>R42C5H11+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 756 CW
R76C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 757 CN
R77C8H16OOH=>R3O2H+C8H16Y    8.5E+12  0.0  26000.0  ! DE 758 CR
R77C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 759 CN
     DUPLICATE
R77C8H16OOH=>R4CH3+C7H13OOHY    6.0E+13  0.0  31000.0  ! DE 760 CN
     DUPLICATE
R78C8H16OOH=>R144C4H8OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 761 CW
R78C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 762 CN
R80C8H16OOH=>R3O2H+C8H16Y    8.5E+12  0.0  26000.0  ! DE 763 CR
R80C8H16OOH=>R40C4H9+C4H7OOHY    2.0E+13  0.0  26700.0  ! DE 764 CW
R81C8H16OOH=>R42C5H11+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 765 CW
R82C8H16OOH=>R4CH3+C7H13OOHY    6.0E+13  0.0  31000.0  ! DE 766 CN
     DUPLICATE
R82C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 767 CN
     DUPLICATE
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R83C8H16OOH=>R135C4H8OOH+C4H8Y    2.0E+13  0.0  28700.0  ! DE 768 CW
R83C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 769 CN
R90C4H8OOH=>R2OH+C3H7CHO    1.0E+09  0.0  7500.0  ! DE 770 CW
R94C7H14OOH=>R11C2H5+C5H9OOHZ    4.0E+13  0.0  28700.0  ! DE 771 CW
R94C7H14OOH=>R2OH+C6H14CO    2.0E+09  0.0  7500.0  ! DE 772 CW
R95C5H10OOH=>R3O2H+C5H10Y    8.5E+12  0.0  26000.0  ! DE 773 CR
R98C5H10OOH=>R2OH+C4H9CHO    1.0E+09  0.0  7500.0  ! DE 774 CW
R101C3H6OOH=>R2OH+C2H5CHO    1.0E+09  0.0  7500.0  ! DE 775 CW
R103C7H14OOH=>R4CH3+C6H11OOHZ    2.0E+13  0.0  31000.0  ! DE 776 CN
R103C7H14OOH=>R19C3H7+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 777 CW
R103C7H14OOH=>R2OH+C6H14CO    1.0E+09  0.0  7500.0  ! DE 778 CW
R104C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 779 CR
R106C5H10OOH=>R101C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 780 CW
R108C7H14OOH=>R184C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 781 CW
R112C7H14OOH=>R20C4H9+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 782 CW
R112C7H14OOH=>R2OH+C6H14CO    1.0E+09  0.0  7500.0  ! DE 783 CW
R113C3H6OOH=>R3O2H+C3H6Y    8.5E+12  0.0  26000.0  ! DE 784 CR
R117C7H14OOH=>R47C4H8OOH+C3H6Y    2.0E+13  0.0  28700.0  ! DE 785 CW
R118C7H14OOH=>R126C5H10OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 786 CW
R121C7H14OOH=>R2OH+C6H13CHO    1.0E+09  0.0  7500.0  ! DE 787 CW
R123C5H10OOH=>R3O2H+C5H10Y    8.5E+12  0.0  26000.0  ! DE 788 CR
R123C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 789 CW
R124C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 790 CN
R125C5H10OOH=>R16C2H4O2H+C3H6Y    2.0E+13  0.0  28700.0  ! DE 791 CW
R126C5H10OOH=>R44C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 792 CW
R131C8H16OOH=>R37C4H9+C4H7OOHY    2.0E+13  0.0  28700.0  ! DE 793 CW
R131C8H16OOH=>R4CH3+C7H13OOHY    4.0E+13  0.0  31000.0  ! DE 794 CN
R131C8H16OOH=>R2OH+C7H15CHO    1.0E+09  0.0  7500.0  ! DE 795 CW
R132C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 796 CR
R134C5H10OOH=>R4CH3+C4H7OOHY    4.0E+13  0.0  31000.0  ! DE 797 CN
R135C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 798 CN
R138C5H10OOH=>R4CH3+C4H7OOHY    6.0E+13  0.0  31000.0  ! DE 799 CN
R138C5H10OOH=>R2OH+C4H9CHO    1.0E+09  0.0  7500.0  ! DE 800 CW
R140C4H8OOH=>R4CH3+C3H5OOHY    4.0E+13  0.0  31000.0  ! DE 801 CN
R140C4H8OOH=>R2OH+C3H7CHO    1.0E+09  0.0  7500.0  ! DE 802 CW
R144C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 803 CR
R144C4H8OOH=>R4CH3+C3H5OOHY    4.0E+13  0.0  31000.0  ! DE 804 CN
R149C8H16OOH=>R42C5H11+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 805 CW
R149C8H16OOH=>R4CH3+C7H13OOHY    2.0E+13  0.0  31000.0  ! DE 806 CN
R149C8H16OOH=>R2OH+C7H15CHO    1.0E+09  0.0  7500.0  ! DE 807 CW
R151C3H5O4H2=>R2OH+C2H4CHOOOH    1.0E+09  0.0  7500.0  ! DE 808 CW
R154C3H5O4H2=>R2OH+C2H4CHOOOH    1.0E+09  0.0  7500.0  ! DE 809 CW
R155C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 810 CW
R161C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 811 CW
R164C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 812 CW
R167C7H13O4H2=>R301C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 813 CW
R168C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 814 CW
R171C7H13O4H2=>R302C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 815 CW
R174C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 816 CW
R179C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 817 CW
R184C5H10OOH=>R113C3H6OOH+C2H4Z    2.0E+13  0.0  28700.0  ! DE 818 CW
R186C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 819 CW
R189C7H13O4H2=>R313C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 820 CW
R191C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 821 CW
R195C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 822 CW
R197C7H13O4H2=>R318C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 823 CW
R199C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 824 CW
R204C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 825 CW
R211C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 826 CW
R214C5H10OOH=>R3O2H+C5H10Y    8.5E+12  0.0  26000.0  ! DE 827 CR
R214C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 828 CW
R215C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 829 CW
R220C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 830 CW
R221C7H13O4H2=>R340C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 831 CW
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R222C7H13O4H2=>R341C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 832 CW
R223C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 833 CW
R224C7H13O4H2=>R342C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 834 CW
R225C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 835 CW
R231C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 836 CW
R232C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 837 CW
R236C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 838 CW
R240C7H13O4H2=>R353C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 839 CW
R241C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 840 CW
R244C7H13O4H2=>R358C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 841 CW
R245C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 842 CW
R250C5H10OOH=>R3O2H+C5H10Y    8.5E+12  0.0  26000.0  ! DE 843 CR
R250C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 844 CN
     DUPLICATE
R250C5H10OOH=>R4CH3+C4H7OOHY    2.0E+13  0.0  31000.0  ! DE 845 CN
     DUPLICATE
R252C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 846 CW
R254C8H15O4H2=>R364C4H7O4H2+C4H8Y    2.0E+13  0.0  28700.0  ! DE 847 CW
R255C8H15O4H2=>R365C5H9O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 848 CW
R257C8H15O4H2=>R366C5H9O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 849 CW
R259C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 850 CW
R263C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 851 CW
R270C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 852 CW
R274C8H15O4H2=>R2OH+C7H15COOOH    1.0E+09  0.0  7500.0  ! DE 853 CW
R278C8H15O4H2=>R2OH+C7H15COOOH    1.0E+09  0.0  7500.0  ! DE 854 CW
R281C8H15O4H2=>R2OH+C7H15COOOH    1.0E+09  0.0  7500.0  ! DE 855 CW
R287C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 856 CW
R289C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 857 CW
R292C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 858 CW
R293C8H15O4H2=>R2OH+C7H14CHOOOH    1.0E+09  0.0  7500.0  ! DE 859 CW
R295C3H5O4H2=>R2OH+C2H5COOOH    1.0E+09  0.0  7500.0  ! DE 860 CW
R296C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 861 CW
R297C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 862 CW
R301C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 863 CW
R305C7H13O4H2=>R384C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 864 CW
R306C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 865 CW
R312C5H10OOH=>R11C2H5+C3H5OOHY    2.0E+13  0.0  28700.0  ! DE 866 CW
R312C5H10OOH=>R2OH+C4H10CO    1.0E+09  0.0  7500.0  ! DE 867 CW
R318C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 868 CW
R324C7H13O4H2=>R391C3H5O4H2+C4H8Y    2.0E+13  0.0  28700.0  ! DE 869 CW
R325C7H13O4H2=>R392C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 870 CW
R326C7H13O4H2=>R393C5H9O4H2+C2H4Z    2.0E+13  0.0  28700.0  ! DE 871 CW
R327C4H8OOH=>R3O2H+C4H8Y    8.5E+12  0.0  26000.0  ! DE 872 CR
R327C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 873 CN
R328C4H9=>R4CH3+C3H6Y    2.0E+13  0.0  31000.0  ! DE 874 CN
R330C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 875 CW
R333C5H11=>R4CH3+C4H8Y    4.0E+13  0.0  31000.0  ! DE 876 CN
R342C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 877 CW
R346C7H13O4H2=>R399C3H5O4H2+C4H8Y    2.0E+13  0.0  28700.0  ! DE 878 CW
R347C7H13O4H2=>R400C4H7O4H2+C3H6Y    2.0E+13  0.0  28700.0  ! DE 879 CW
R358C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 880 CW
R366C5H9O4H2=>R2OH+C4H8CHOOOH    1.0E+09  0.0  7500.0  ! DE 881 CW
R372C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 882 CW
R374C4H7O4H2=>R2OH+C3H6CHOOOH    1.0E+09  0.0  7500.0  ! DE 883 CW
R382C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 884 CW
R386C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 885 CW
R387C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 886 CW
R390C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 887 CW
R391C3H5O4H2=>R2OH+C2H5COOOH    1.0E+09  0.0  7500.0  ! DE 888 CW
R394C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 889 CW
R395C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 890 CW
R396C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 891 CW
R397C5H9O4H2=>R2OH+C4H9COOOH    1.0E+09  0.0  7500.0  ! DE 892 CW
R401C7H13O4H2=>R2OH+C6H12CHOOOH    1.0E+09  0.0  7500.0  ! DE 893 CW
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R404C7H13O4H2=>R2OH+C6H13COOOH    1.0E+09  0.0  7500.0  ! DE 894 CW
R405C8H15O4H2=>R2OH+C7H15COOOH    1.0E+09  0.0  7500.0  ! DE 895 CW
R406C8H15O4H2=>R2OH+C7H15COOOH    1.0E+09  0.0  7500.0  ! DE 896 CW
R410C4H7O4H2=>R2OH+C3H7COOOH    1.0E+09  0.0  7500.0  ! DE 897 CW
R416C4H8OOH=>R2OH+C3H8CO    1.0E+09  0.0  7500.0  ! DE 898 CW
R416C4H8OOH=>R4CH3+C3H5OOHY    2.0E+13  0.0  31000.0  ! DE 899 CN
R417C5H10OOH=>R4CH3+C4H7OOHY    4.0E+13  0.0  31000.0  ! DE 900 CN
R417C5H10OOH=>R2OH+C4H10CO    2.0E+09  0.0  7500.0  ! DE 901 CW
R418C3H6OOH=>R2OH+C2H6CO    2.0E+09  0.0  7500.0  ! DE 902 CW

!   decomposition to o-rings :
R43C3H6OOH=>R2OH+C3H6O#3    1.0E+12  0.0  16500.0  ! OR 903 CR
R44C3H6OOH=>R2OH+C3H6O#4    2.0E+11  0.0  15500.0  ! OR 904 CR
R45C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 905 CR
R46C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 906 CR
R47C4H8OOH=>R2OH+C4H8O#5    6.0E+10  0.0  9000.0  ! OR 907 CR
R48C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 908 CR
R49C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 909 CR
R50C7H14OOH=>R2OH+C7H14O#5    6.0E+10  0.0  9000.0  ! OR 910 CR
R51C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 911 CR
R52C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 912 CR
R53C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 913 CR
R54C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 914 CR
R55C7H14OOH=>R2OH+C7H14O#5    6.0E+10  0.0  9000.0  ! OR 915 CR
R56C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 916 CN
R57C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 917 CR
R58C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 918 CR
R59C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 919 CR
R60C7H14OOH=>R2OH+C7H14O#5    6.0E+10  0.0  9000.0  ! OR 920 CR
R61C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 921 CN
R62C7H14OOH=>R2OH+C7H14O#3    1.0E+12  0.0  16500.0  ! OR 922 CR
R63C7H14OOH=>R2OH+C7H14O#4    2.0E+11  0.0  15500.0  ! OR 923 CR
R64C7H14OOH=>R2OH+C7H14O#5    6.0E+10  0.0  9000.0  ! OR 924 CR
R65C7H14OOH=>R2OH+C7H14O#6    1.0E+10  0.0  6000.0  ! OR 925 CN
R68C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 926 CR
R69C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 927 CR
R70C8H16OOH=>R2OH+C8H16O#5    6.0E+10  0.0  9000.0  ! OR 928 CR
R71C8H16OOH=>R2OH+C8H16O#6    1.0E+10  0.0  6000.0  ! OR 929 CN
R73C8H16OOH=>R2OH+C8H16O#3    1.0E+12  0.0  16500.0  ! OR 930 CR
R74C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 931 CR
R75C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 932 CR
R76C8H16OOH=>R2OH+C8H16O#3    1.0E+12  0.0  16500.0  ! OR 933 CR
R77C8H16OOH=>R2OH+C8H16O#3    1.0E+12  0.0  16500.0  ! OR 934 CR
R78C8H16OOH=>R2OH+C8H16O#5    6.0E+10  0.0  9000.0  ! OR 935 CR
R80C8H16OOH=>R2OH+C8H16O#3    1.0E+12  0.0  16500.0  ! OR 936 CR
R81C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 937 CR
R82C8H16OOH=>R2OH+C8H16O#4    2.0E+11  0.0  15500.0  ! OR 938 CR
R83C8H16OOH=>R2OH+C8H16O#6    1.0E+10  0.0  6000.0  ! OR 939 CN
R95C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 940 CR
R104C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 941 CR
R106C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 942 CR
R113C3H6OOH=>R2OH+C3H6O#3    1.0E+12  0.0  16500.0  ! OR 943 CR
R115C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 944 CR
R123C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 945 CR
R124C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 946 CR
R125C5H10OOH=>R2OH+C5H10O#5    6.0E+10  0.0  9000.0  ! OR 947 CR
R126C5H10OOH=>R2OH+C5H10O#6    1.0E+10  0.0  6000.0  ! OR 948 CN
R132C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 949 CR
R134C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 950 CR
R135C4H8OOH=>R2OH+C4H8O#4    2.0E+11  0.0  15500.0  ! OR 951 CR
R144C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 952 CR
R150C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 953 CR
R150C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 954 CR
R151C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 955 CR
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R153C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 956 CR
R154C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 957 CR
R155C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 958 CR
R157C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 959 CR
R157C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 960 CR
R158C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 961 CR
R158C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+10  0.0  9000.0  ! OR 962 CR
R159C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 963 CR
R159C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+10  0.0  9000.0  ! OR 964 CR
R160C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 965 CR
     DUPLICATE
R160C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 966 CR
     DUPLICATE
R161C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 967 CR
R163C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 968 CR
R163C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 969 CR
R164C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+10  0.0  9000.0  ! OR 970 CR
R166C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 971 CR
R166C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 972 CR
R167C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 973 CR
R167C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 974 CR
R168C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 975 CR
R169C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 976 CR
R169C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 977 CR
R170C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 978 CR
R170C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 979 CR
R171C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 980 CR
R171C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 981 CN
R172C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 982 CR
R172C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 983 CR
R173C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 984 CR
     DUPLICATE
R173C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 985 CR
     DUPLICATE
R174C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 986 CR
R175C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 987 CR
R175C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 988 CR
R176C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 989 CR
R176C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 990 CN
R177C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 991 CR
R177C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 992 CR
R178C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 993 CR
R178C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 994 CR
R179C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 995 CR
R180C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 996 CR
R180C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 997 CN
R183C5H10OOH=>R2OH+C5H10O#4    2.0E+11  0.0  15500.0  ! OR 998 CR
R184C5H10OOH=>R2OH+C5H10O#5    6.0E+10  0.0  9000.0  ! OR 999 CR
R185C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1000 CR
R185C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1001 CR
R186C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1002 CR
R187C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1003 CR
R187C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1004 CR
R188C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1005 CR
R188C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1006 CR
R189C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1007 CR
R189C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1008 CN
R190C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1009 CR
     DUPLICATE
R190C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1010 CR
     DUPLICATE
R191C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1011 CR
R192C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1012 CR
R192C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1013 CR
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R193C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1014 CR
R193C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1015 CN
R195C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1016 CR
R196C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1017 CR
R196C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1018 CR
R197C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1019 CR
R197C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1020 CN
R198C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1021 CR
R199C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1022 CR
R201C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1023 CR
R201C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1024 CN
R202C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1025 CR
R202C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1026 CR
R203C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1027 CR
R203C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1028 CR
R204C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1029 CR
R205C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1030 CR
R205C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1031 CN
R208C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1032 CR
R208C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1033 CR
R209C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1034 CR
     DUPLICATE
R209C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1035 CR
     DUPLICATE
R210C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1036 CR
R210C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1037 CR
R211C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1038 CN
R214C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 1039 CR
R215C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1040 CR
R216C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1041 CR
R216C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1042 CR
R217C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1043 CR
R217C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1044 CR
R218C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1045 CR
R218C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1046 CN
R220C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1047 CR
R221C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1048 CN
R222C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1049 CR
R223C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1050 CR
R224C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1051 CR
R225C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1052 CR
R228C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1053 CR
R229C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1054 CR
R229C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1055 CR
R230C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1056 CR
R231C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1057 CN
R232C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1058 CR
R233C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1059 CN
R236C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1060 CR
R237C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1061 CR
R238C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1062 CN
R239C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1063 CR
R240C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1064 CR
R241C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1065 CR
R243C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1066 CR
R244C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1067 CR
R245C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1068 CN
R250C5H10OOH=>R2OH+C5H10O#3    1.0E+12  0.0  16500.0  ! OR 1069 CR
R251C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1070 CR
R252C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1071 CR
R253C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1072 CR
R254C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1073 CR
R255C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1074 CN
R256C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1075 CR
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R256C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1076 CR
R257C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1077 CR
R257C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1078 CN
R258C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1079 CR
     DUPLICATE
R258C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1080 CR
     DUPLICATE
R259C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1081 CR
R260C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1082 CR
R260C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1083 CN
R261C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1084 CR
R261C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1085 CR
R262C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1086 CR
R262C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1087 CR
R263C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1088 CR
R266C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1089 CR
R266C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1090 CR
R267C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1091 CR
R267C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1092 CN
R268C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1093 CR
     DUPLICATE
R268C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1094 CR
     DUPLICATE
R269C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1095 CR
R269C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1096 CN
R270C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1097 CN
R273C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1098 CR
R273C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1099 CR
R274C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1100 CR
R275C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1101 CR
R275C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1102 CR
R276C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1103 CR
     DUPLICATE
R276C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1104 CR
     DUPLICATE
R277C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1105 CR
     DUPLICATE
R277C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1106 CR
     DUPLICATE
R278C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1107 CR
R279C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1108 CR
R279C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1109 CN
R281C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1110 CR
R283C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1111 CR
R283C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1112 CR
R284C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1113 CR
R284C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1114 CR
R285C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1115 CR
R285C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1116 CN
R287C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1117 CR
R288C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1118 CR
R289C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1119 CR
R290C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1120 CR
R291C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1121 CN
R292C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1122 CR
R293C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1123 CN
R295C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1124 CR
R296C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1125 CR
R297C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1126 CR
R298C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1127 CR
R299C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1128 CR
R300C4H7O4H2=>R2OH+C4H7O#5OOH    6.0E+10  0.0  9000.0  ! OR 1129 CR
R301C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1130 CR
R302C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1131 CR
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R302C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1132 CR
R303C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1133 CR
R304C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1134 CR
R305C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1135 CR
R306C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1136 CR
R307C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1137 CR
R307C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1138 CR
R308C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1139 CR
R308C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1140 CR
R309C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1141 CR
R309C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1142 CN
R313C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1143 CR
R313C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1144 CR
R314C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1145 CR
R315C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1146 CR
R316C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1147 CR
R317C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1148 CN
R318C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1149 CR
R319C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1150 CR
R320C3H5O4H2=>R2OH+C3H5O#4OOH    2.0E+11  0.0  15500.0  ! OR 1151 CR
R321C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1152 CR
R322C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1153 CR
R323C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1154 CR
R324C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1155 CR
R325C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1156 CR
R326C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1157 CN
R327C4H8OOH=>R2OH+C4H8O#3    1.0E+12  0.0  16500.0  ! OR 1158 CR
R329C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1159 CR
     DUPLICATE
R329C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1160 CR
     DUPLICATE
R330C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1161 CR
R331C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1162 CR
R331C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1163 CR
R332C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1164 CR
R332C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1165 CN
R336C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1166 CR
R336C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1167 CN
R337C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1168 CR
R337C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1169 CR
R338C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1170 CR
R338C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1171 CR
R339C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1172 CR
R339C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1173 CN
R340C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1174 CR
R340C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1175 CR
R341C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1176 CR
R341C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1177 CR
R342C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1178 CR
R343C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1179 CR
R344C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1180 CR
R345C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1181 CR
R346C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1182 CR
R347C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1183 CN
R349C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1184 CR
R350C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1185 CR
R351C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1186 CR
R351C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1187 CN
R352C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1188 CR
R353C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1189 CR
R353C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1190 CN
R354C7H13O4H2=>R2OH+C7H13O#3OOH    1.0E+12  0.0  16500.0  ! OR 1191 CR
R355C7H13O4H2=>R2OH+C7H13O#4OOH    2.0E+11  0.0  15500.0  ! OR 1192 CR
R356C7H13O4H2=>R2OH+C7H13O#5OOH    6.0E+10  0.0  9000.0  ! OR 1193 CR
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R357C7H13O4H2=>R2OH+C7H13O#6OOH    1.0E+10  0.0  6000.0  ! OR 1194 CN
R358C5H9O4H2=>R2OH+C5H9O#6OOH    1.0E+10  0.0  6000.0  ! OR 1195 CN
R359C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1196 CR
R359C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1197 CR
R360C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1198 CR
R360C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1199 CR
R361C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1200 CR
R361C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1201 CR
R362C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1202 CR
R364C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1203 CR
R365C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1204 CR
R366C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1205 CR
R367C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1206 CR
R368C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1207 CR
R369C8H15O4H2=>R2OH+C8H15O#5OOH    6.0E+10  0.0  9000.0  ! OR 1208 CR
R370C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1209 CN
R371C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1210 CR
R371C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1211 CR
R372C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1212 CR
R373C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1213 CR
R374C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1214 CR
R375C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1215 CR
R376C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1216 CR
R377C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1217 CR
R378C8H15O4H2=>R2OH+C8H15O#3OOH    1.0E+12  0.0  16500.0  ! OR 1218 CR
R379C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1219 CR
R380C8H15O4H2=>R2OH+C8H15O#4OOH    2.0E+11  0.0  15500.0  ! OR 1220 CR
R381C8H15O4H2=>R2OH+C8H15O#6OOH    1.0E+10  0.0  6000.0  ! OR 1221 CN
R383C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1222 CR
R383C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1223 CR
R384C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1224 CR
R385C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1225 CR
R386C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1226 CR
R387C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1227 CR
R392C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1228 CR
R393C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1229 CR
R394C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1230 CR
R397C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1231 CR
R399C3H5O4H2=>R2OH+C3H5O#3OOH    1.0E+12  0.0  16500.0  ! OR 1232 CR
R400C4H7O4H2=>R2OH+C4H7O#4OOH    2.0E+11  0.0  15500.0  ! OR 1233 CR
R407C5H9O4H2=>R2OH+C5H9O#4OOH    2.0E+11  0.0  15500.0  ! OR 1234 CR
R408C5H9O4H2=>R2OH+C5H9O#5OOH    6.0E+10  0.0  9000.0  ! OR 1235 CR
R409C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1236 CR
R410C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1237 CR
R413C5H9O4H2=>R2OH+C5H9O#3OOH    1.0E+12  0.0  16500.0  ! OR 1238 CR
R415C4H7O4H2=>R2OH+C4H7O#3OOH    1.0E+12  0.0  16500.0  ! OR 1239 CR

!   oxidations :
R21C7H15+O2=>C7H14Y+R3O2H    3.2E+12  0.0  5000.0  ! OX 1240 CN
R22C7H15+O2=>C7H14Y+R3O2H    1.6E+12  0.0  5000.0  ! OX 1241 CN
     DUPLICATE
R22C7H15+O2=>C7H14Y+R3O2H    1.6E+12  0.0  5000.0  ! OX 1242 CN
     DUPLICATE
R23C7H15+O2=>C7H14Y+R3O2H    6.9E+11  0.0  5000.0  ! OX 1243 CN
     DUPLICATE
R23C7H15+O2=>C7H14Y+R3O2H    1.6E+12  0.0  5000.0  ! OX 1244 CN
     DUPLICATE
R24C7H15+O2=>C7H14Y+R3O2H    1.6E+12  0.0  5000.0  ! OX 1245 CN
R26C8H17+O2=>C8H16Y+R3O2H    4.5E+11  0.0  5000.0  ! OX 1246 CN
R27C8H17+O2=>C8H16Y+R3O2H    1.4E+12  0.0  5000.0  ! OX 1247 CN
     DUPLICATE
R27C8H17+O2=>C8H16Y+R3O2H    1.6E+12  0.0  5000.0  ! OX 1248 CN
     DUPLICATE
R28C8H17+O2=>C8H16Y+R3O2H    4.5E+11  0.0  5000.0  ! OX 1249 CN
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R40C4H9+O2=>C4H8Y+R3O2H    2.1E+12  0.0  5000.0  ! OX 1250 CN
R348C3H7+O2=>C3H6Y+R3O2H    1.4E+12  0.0  5000.0  ! OX 1251 CN

!   metathesis :
B1O+C7H16=>R2OH+R21C7H15    2.6E+13  0.0  5200.0  ! ME 1252 CW
B1O+C7H16=>R2OH+R22C7H15    5.2E+13  0.0  5200.0  ! ME 1253 CW
B1O+C7H16=>R2OH+R23C7H15    5.2E+13  0.0  5200.0  ! ME 1254 CW
B1O+C7H16=>R2OH+R24C7H15    1.0E+14  0.0  7850.0  ! ME 1255 CW
B1O+C8H18=>R2OH+R25C8H17    1.5E+14  0.0  7850.0  ! ME 1256 CW
B1O+C8H18=>R2OH+R26C8H17    2.6E+13  0.0  5200.0  ! ME 1257 CW
B1O+C8H18=>R2OH+R27C8H17    1.0E+13  0.0  3280.0  ! ME 1258 CW
B1O+C8H18=>R2OH+R28C8H17    1.0E+14  0.0  7850.0  ! ME 1259 CW
C7H16+R1H=>H2+R21C7H15    9.0E+06  2.0  5000.0  ! ME 1260 CW
C7H16+R1H=>H2+R22C7H15    1.8E+07  2.0  5000.0  ! ME 1261 CW
C7H16+R1H=>H2+R23C7H15    1.8E+07  2.0  5000.0  ! ME 1262 CW
C7H16+R1H=>H2+R24C7H15    5.6E+07  2.0  7700.0  ! ME 1263 CW
C8H18+R1H=>H2+R25C8H17    8.5E+07  2.0  7700.0  ! ME 1264 CW
C8H18+R1H=>H2+R26C8H17    9.0E+06  2.0  5000.0  ! ME 1265 CW
C8H18+R1H=>H2+R27C8H17    4.2E+06  2.0  2400.0  ! ME 1266 CN
C8H18+R1H=>H2+R28C8H17    5.6E+07  2.0  7700.0  ! ME 1267 CW
C7H16+R2OH=>H2O+R21C7H15    2.6E+06  2.0  -765.0  ! ME 1268 CW
C7H16+R2OH=>H2O+R22C7H15    5.2E+06  2.0  -765.0  ! ME 1269 CW
C7H16+R2OH=>H2O+R23C7H15    5.2E+06  2.0  -765.0  ! ME 1270 CW
C7H16+R2OH=>H2O+R24C7H15    5.4E+06  2.0  450.0  ! ME 1271 CW
C8H18+R2OH=>H2O+R25C8H17    8.1E+06  2.0  450.0  ! ME 1272 CW
C8H18+R2OH=>H2O+R26C8H17    2.6E+06  2.0  -765.0  ! ME 1273 CW
C8H18+R2OH=>H2O+R27C8H17    1.1E+06  2.0  -1865.0  ! ME 1274 CW
C8H18+R2OH=>H2O+R28C8H17    5.4E+06  2.0  450.0  ! ME 1275 CW
C7H16+R3O2H=>H2O2+R21C7H15    4.0E+11  0.0  15500.0  ! ME 1276 CN
C7H16+R3O2H=>H2O2+R22C7H15    8.0E+11  0.0  15500.0  ! ME 1277 CN
C7H16+R3O2H=>H2O2+R23C7H15    8.0E+11  0.0  15500.0  ! ME 1278 CN
C7H16+R3O2H=>H2O2+R24C7H15    1.2E+12  0.0  17000.0  ! ME 1279 CN
C8H18+R3O2H=>H2O2+R25C8H17    1.8E+12  0.0  17000.0  ! ME 1280 CN
C8H18+R3O2H=>H2O2+R26C8H17    4.0E+11  0.0  15500.0  ! ME 1281 CN
C8H18+R3O2H=>H2O2+R27C8H17    1.0E+12  0.0  14000.0  ! ME 1282 CN
C8H18+R3O2H=>H2O2+R28C8H17    1.2E+12  0.0  17000.0  ! ME 1283 CN
C7H16+R4CH3=>CH4+R21C7H15    2.0E+11  0.0  9600.0  ! ME 1284 CN
C7H16+R4CH3=>CH4+R22C7H15    4.0E+11  0.0  9600.0  ! ME 1285 CN
C7H16+R4CH3=>CH4+R23C7H15    4.0E+11  0.0  9600.0  ! ME 1286 CN
C7H16+R4CH3=>CH4+R24C7H15    6.0E-01  4.0  8200.0  ! ME 1287 CN
C8H18+R4CH3=>CH4+R25C8H17    9.0E-01  4.0  8200.0  ! ME 1288 CN
C8H18+R4CH3=>CH4+R26C8H17    2.0E+11  0.0  9600.0  ! ME 1289 CN
C8H18+R4CH3=>CH4+R27C8H17    1.0E+11  0.0  7900.0  ! ME 1290 CW
C8H18+R4CH3=>CH4+R28C8H17    6.0E-01  4.0  8200.0  ! ME 1291 CN
C7H16+R5CHO=>HCHO+R21C7H15    1.1E+07  1.9  17000.0  ! ME 1292 CN
C7H16+R5CHO=>HCHO+R22C7H15    2.2E+07  1.9  17000.0  ! ME 1293 CN
C7H16+R5CHO=>HCHO+R23C7H15    2.2E+07  1.9  17000.0  ! ME 1294 CN
C7H16+R5CHO=>HCHO+R24C7H15    2.0E+05  2.5  18500.0  ! ME 1295 CN
C8H18+R5CHO=>HCHO+R25C8H17    3.1E+05  2.5  18500.0  ! ME 1296 CN
C8H18+R5CHO=>HCHO+R26C8H17    1.1E+07  1.9  17000.0  ! ME 1297 CN
C8H18+R5CHO=>HCHO+R27C8H17    3.4E+04  2.5  13500.0  ! ME 1298 CN
C8H18+R5CHO=>HCHO+R28C8H17    2.0E+05  2.5  18500.0  ! ME 1299 CN
C7H16+R6CH2OH=>CH3OH+R21C7H15    6.0E+01  3.0  12000.0  ! ME 1300 CN
C7H16+R6CH2OH=>CH3OH+R22C7H15    1.2E+02  3.0  12000.0  ! ME 1301 CN
C7H16+R6CH2OH=>CH3OH+R23C7H15    1.2E+02  3.0  12000.0  ! ME 1302 CN
C7H16+R6CH2OH=>CH3OH+R24C7H15    2.0E+02  3.0  14000.0  ! ME 1303 CN
C8H18+R6CH2OH=>CH3OH+R25C8H17    3.0E+02  3.0  14000.0  ! ME 1304 CN
C8H18+R6CH2OH=>CH3OH+R26C8H17    6.0E+01  3.0  12000.0  ! ME 1305 CN
C8H18+R6CH2OH=>CH3OH+R27C8H17    1.2E+02  2.8  10800.0  ! ME 1306 CN
C8H18+R6CH2OH=>CH3OH+R28C8H17    2.0E+02  3.0  14000.0  ! ME 1307 CN
C7H16+R7CH3O=>CH3OH+R21C7H15    1.5E+11  0.0  4500.0  ! ME 1308 CN
C7H16+R7CH3O=>CH3OH+R22C7H15    2.9E+11  0.0  4500.0  ! ME 1309 CN
C7H16+R7CH3O=>CH3OH+R23C7H15    2.9E+11  0.0  4500.0  ! ME 1310 CN
C7H16+R7CH3O=>CH3OH+R24C7H15    3.2E+11  0.0  7300.0  ! ME 1311 CN
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C8H18+R7CH3O=>CH3OH+R25C8H17    4.9E+11  0.0  7300.0  ! ME 1312 CN
C8H18+R7CH3O=>CH3OH+R26C8H17    1.5E+11  0.0  4500.0  ! ME 1313 CN
C8H18+R7CH3O=>CH3OH+R27C8H17    2.3E+10  0.0  2900.0  ! ME 1314 CN
C8H18+R7CH3O=>CH3OH+R28C8H17    3.2E+11  0.0  7300.0  ! ME 1315 CN
C7H16+R8CH3OO=>CH3O2H+R21C7H15    3.0E+12  0.0  17500.0  ! ME 1316 CN
C7H16+R8CH3OO=>CH3O2H+R22C7H15    6.0E+12  0.0  17500.0  ! ME 1317 CN
C7H16+R8CH3OO=>CH3O2H+R23C7H15    6.0E+12  0.0  17500.0  ! ME 1318 CN
C7H16+R8CH3OO=>CH3O2H+R24C7H15    1.2E+13  0.0  20000.0  ! ME 1319 CN
C8H18+R8CH3OO=>CH3O2H+R25C8H17    1.8E+13  0.0  20000.0  ! ME 1320 CN
C8H18+R8CH3OO=>CH3O2H+R26C8H17    3.0E+12  0.0  17500.0  ! ME 1321 CN
C8H18+R8CH3OO=>CH3O2H+R27C8H17    1.5E+12  0.0  15000.0  ! ME 1322 CN
C8H18+R8CH3OO=>CH3O2H+R28C8H17    1.2E+13  0.0  20000.0  ! ME 1323 CN
C7H16+R11C2H5=>C2H6+R21C7H15    2.0E+11  0.0  11000.0  ! ME 1324 CN
C7H16+R11C2H5=>C2H6+R22C7H15    4.0E+11  0.0  11000.0  ! ME 1325 CN
C7H16+R11C2H5=>C2H6+R23C7H15    4.0E+11  0.0  11000.0  ! ME 1326 CN
C7H16+R11C2H5=>C2H6+R24C7H15    6.0E+11  0.0  13500.0  ! ME 1327 CR
C8H18+R11C2H5=>C2H6+R25C8H17    9.0E+11  0.0  13500.0  ! ME 1328 CR
C8H18+R11C2H5=>C2H6+R26C8H17    2.0E+11  0.0  11000.0  ! ME 1329 CN
C8H18+R11C2H5=>C2H6+R27C8H17    1.0E+11  0.0  9200.0  ! ME 1330 CN
C8H18+R11C2H5=>C2H6+R28C8H17    6.0E+11  0.0  13500.0  ! ME 1331 CR
C7H16+R40C4H9=>C4H10+R21C7H15    2.0E+11  0.0  12700.0  ! ME 1332 CR
C7H16+R40C4H9=>C4H10+R22C7H15    4.0E+11  0.0  12700.0  ! ME 1333 CR
C7H16+R40C4H9=>C4H10+R23C7H15    4.0E+11  0.0  12700.0  ! ME 1334 CR
C7H16+R40C4H9=>C4H10+R24C7H15    6.0E+11  0.0  15000.0  ! ME 1335 CR
C8H18+R40C4H9=>C4H10+R25C8H17    9.0E+11  0.0  15000.0  ! ME 1336 CR
C8H18+R40C4H9=>C4H10+R26C8H17    2.0E+11  0.0  12700.0  ! ME 1337 CR
C8H18+R40C4H9=>C4H10+R27C8H17    1.0E+11  0.0  10500.0  ! ME 1338 CR
C8H18+R40C4H9=>C4H10+R28C8H17    6.0E+11  0.0  15000.0  ! ME 1339 CR
C7H16+R348C3H7=>C3H8+R21C7H15    2.8E-03  4.2  8000.0  ! ME 1340 CN
C7H16+R348C3H7=>C3H8+R22C7H15    5.6E-03  4.2  8000.0  ! ME 1341 CN
C7H16+R348C3H7=>C3H8+R23C7H15    5.6E-03  4.2  8000.0  ! ME 1342 CN
C7H16+R348C3H7=>C3H8+R24C7H15    8.4E-03  4.2  8700.0  ! ME 1343 CN
C8H18+R348C3H7=>C3H8+R25C8H17    1.3E-02  4.2  8700.0  ! ME 1344 CN
C8H18+R348C3H7=>C3H8+R26C8H17    2.8E-03  4.2  8000.0  ! ME 1345 CN
C8H18+R348C3H7=>C3H8+R27C8H17    1.4E-03  4.2  6000.0  ! ME 1346 CN
C8H18+R348C3H7=>C3H8+R28C8H17    8.4E-03  4.2  8700.0  ! ME 1347 CN

C7H16+R25C8H17=>C8H18+R21C7H15    2.0E+11  0.0  11200.0  ! ME 1332 CR
C7H16+R25C8H17=>C8H18+R22C7H15    4.0E+11  0.0  11200.0  ! ME 1333 CR
C7H16+R25C8H17=>C8H18+R23C7H15    4.0E+11  0.0  11200.0  ! ME 1334 CR
C7H16+R25C8H17=>C8H18+R24C7H15    6.0E+11  0.0  13500.0  ! ME 1335 CR
C7H16+R26C8H17=>C8H18+R21C7H15    2.0E+11  0.0  12200.0  ! ME 1332 CR
C7H16+R26C8H17=>C8H18+R22C7H15    4.0E+11  0.0  12200.0  ! ME 1333 CR
C7H16+R26C8H17=>C8H18+R23C7H15    4.0E+11  0.0  12200.0  ! ME 1334 CR
C7H16+R26C8H17=>C8H18+R24C7H15    6.0E+11  0.0  14500.0  ! ME 1335 CR
C7H16+R27C8H17=>C8H18+R21C7H15    2.0E+11  0.0  12700.0  ! ME 1332 CR
C7H16+R27C8H17=>C8H18+R22C7H15    4.0E+11  0.0  12700.0  ! ME 1333 CR
C7H16+R27C8H17=>C8H18+R23C7H15    4.0E+11  0.0  12700.0  ! ME 1334 CR
C7H16+R27C8H17=>C8H18+R24C7H15    6.0E+11  0.0  15000.0  ! ME 1335 CR
C7H16+R28C8H17=>C8H18+R21C7H15    2.0E+11  0.0  11200.0  ! ME 1332 CR
C7H16+R28C8H17=>C8H18+R22C7H15    4.0E+11  0.0  11200.0  ! ME 1333 CR
C7H16+R28C8H17=>C8H18+R23C7H15    4.0E+11  0.0  11200.0  ! ME 1334 CR
C7H16+R28C8H17=>C8H18+R24C7H15    6.0E+11  0.0  13500.0  ! ME 1335 CR
C8H18+R21C7H15=>C7H16+R25C8H17    9.0E+11  0.0  14500.0  ! ME 1344 CN
C8H18+R21C7H15=>C7H16+R26C8H17    2.0E+11  0.0  11200.0  ! ME 1345 CN
C8H18+R21C7H15=>C7H16+R27C8H17    1.0E+11  0.0  10000.0  ! ME 1346 CN
C8H18+R21C7H15=>C7H16+R28C8H17    6.0E+11  0.0  14500.0  ! ME 1347 CN
C8H18+R22C7H15=>C7H16+R25C8H17    9.0E+11  0.0  14500.0  ! ME 1344 CN
C8H18+R22C7H15=>C7H16+R26C8H17    2.0E+11  0.0  11200.0  ! ME 1345 CN
C8H18+R22C7H15=>C7H16+R27C8H17    1.0E+11  0.0  10000.0  ! ME 1346 CN
C8H18+R22C7H15=>C7H16+R28C8H17    6.0E+11  0.0  14500.0  ! ME 1347 CN
C8H18+R23C7H15=>C7H16+R25C8H17    9.0E+11  0.0  14500.0  ! ME 1344 CN
C8H18+R23C7H15=>C7H16+R26C8H17    2.0E+11  0.0  11200.0  ! ME 1345 CN
C8H18+R23C7H15=>C7H16+R27C8H17    1.0E+11  0.0  10000.0  ! ME 1346 CN
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C8H18+R23C7H15=>C7H16+R28C8H17    6.0E+11  0.0  14500.0  ! ME 1347 CN
C8H18+R24C7H15=>C7H16+R25C8H17    9.0E+11  0.0  13500.0  ! ME 1344 CN
C8H18+R24C7H15=>C7H16+R26C8H17    2.0E+11  0.0  11200.0  ! ME 1345 CN
C8H18+R24C7H15=>C7H16+R27C8H17    1.0E+11  0.0   9000.0  ! ME 1346 CN
C8H18+R24C7H15=>C7H16+R28C8H17    6.0E+11  0.0  13500.0  ! ME 1347 CN

!   combinations :
R1H+R40C4H9=>C4H10    9.2E+12  0.0  0.0  ! CO 1348 KB
R1H+R348C3H7=>C3H8    9.2E+12  0.0  0.0  ! CO 1349 KB
R2OH+R40C4H9=>C4H9OH    6.2E+12  0.0  0.0  ! CO 1350 KB
R2OH+R348C3H7=>C3H7OH    6.4E+12  0.0  0.0  ! CO 1351 KB
R3O2H+R40C4H9=>C4H9OOH    4.9E+12  0.0  0.0  ! CO 1352 KB
R3O2H+R348C3H7=>C3H7OOH    5.2E+12  0.0  0.0  ! CO 1353 KB
R4CH3+R40C4H9=>C5H12    1.7E+13  0.0  0.0  ! CO 1354 KB
R4CH3+R348C3H7=>C4H10    1.7E+13  0.0  0.0  ! CO 1355 KB
R5CHO+R40C4H9=>C4H9CHO    5.3E+12  0.0  0.0  ! CO 1356 KB
R5CHO+R348C3H7=>C3H7CHO    5.6E+12  0.0  0.0  ! CO 1357 KB
R6CH2OH+R40C4H9=>C5H11OH    5.2E+12  0.0  0.0  ! CO 1358 KB
R6CH2OH+R348C3H7=>C4H9OH    5.5E+12  0.0  0.0  ! CO 1359 KB
R7CH3O+R40C4H9=>C5H12O    5.0E+12  0.0  0.0  ! CO 1360 KB
R7CH3O+R348C3H7=>C4H10O    5.3E+12  0.0  0.0  ! CO 1361 KB
R11C2H5+R40C4H9=>C6H14    5.3E+12  0.0  0.0  ! CO 1362 KB
R11C2H5+R348C3H7=>C5H12    5.6E+12  0.0  0.0  ! CO 1363 KB
R40C4H9+R40C4H9=>C8H18    2.2E+12  0.0  0.0  ! CO 1364 KB
R40C4H9+R348C3H7=>C7H16    4.7E+12  0.0  0.0  ! CO 1365 KB
R348C3H7+R348C3H7=>C6H14    2.5E+12  0.0  0.0  ! CO 1366 KB

!   dismutations :
R29C3H7OO+R3O2H=>C3H7OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1367 CN
R30C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1368 CN
R31C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1369 CN
R32C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1370 CN
R33C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1371 CN
R34C7H15OO+R3O2H=>C7H15OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1372 CN
R36C8H17OO+R3O2H=>C8H17OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1373 CN
R38C8H17OO+R3O2H=>C8H17OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1374 CN
R39C8H17OO+R3O2H=>C8H17OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1375 CN
R41C8H17OO+R3O2H=>C8H17OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1376 CN
R66C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1377 CN
R72C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1378 CN
R79C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1379 CN
R84C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1380 CN
R127C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1381 CN
R207C4H9OO+R3O2H=>C4H9OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1382 CN
R213C5H11OO+R3O2H=>C5H11OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1383 CN
R227C3H7OO+R3O2H=>C3H7OOH+O2    2.0E+11  0.0  -1300.0  ! DI 1384 CN

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

! Hydroperoxide decomposition
C3H5OOHY=>R2OH+HCHO+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 2066
C6H11OOHZ=>R2OH+CH3CHO+C2H4Z+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 2067
C4H7OOHY=>R2OH+CH3CHO+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 2068
C5H9OOHZ=>R2OH+HCHO+C2H4Z+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 2069
C7H13OOHY=>R2OH+HCHO+2C2H4Z+R10C2H3V    7.0E+14  0.0  42000.0  ! DKH 2070
C4H9OOH=>R2OH+CH3CHO+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 2071
C3H7OOH=>R2OH+HCHO+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 2072
C7H15OOH=>R2OH+HCHO+2C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 2073
C8H17OOH=>R2OH+CH3CHO+2C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 2074
C5H11OOH=>R2OH+HCHO+C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DKH 2075

! Dihydroperoxide decomposition
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! Ketohydroperoxide decomposition
C6H13COOOH=>R2OH+HCHO+B2CO+2C2H4Z+R4CH3    7.0E+14  0.0  42000.0  ! DK1 2076
C7H15COOOH=>R2OH+HCHO+B2CO+2C2H4Z+R11C2H5    7.0E+14  0.0  42000.0  ! DK1 2077
C2H5COOOH=>R2OH+HCHO+B2CO+R4CH3    7.0E+14  0.0  42000.0  ! DK1 2078
C3H7COOOH=>R2OH+HCHO+B2CO+R11C2H5    7.0E+14  0.0  42000.0  ! DK1 2079
C4H9COOOH=>R2OH+HCHO+B2CO+C2H4Z+R4CH3    7.0E+14  0.0  42000.0  ! DK1 2080

! Aldohydroperoxide decomposition
C2H4CHOOOH=>R2OH+CH3CHO+R5CHO    7.0E+14  0.0  42000.0  ! DK2 2081
C3H6CHOOOH=>R2OH+CH3CHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DK2 2082
C6H12CHOOOH=>R2OH+CH3CHO+2C2H4Z+R5CHO    7.0E+14  0.0  42000.0  ! DK2 2083
C7H14CHOOOH=>R2OH+CH3CHO+2C2H4Z+R13CH2CHO    7.0E+14  0.0  42000.0  ! DK2 2084
C4H8CHOOOH=>R2OH+CH3CHO+C2H4Z+R5CHO    7.0E+14  0.0  42000.0  ! DK2 2085

! Hydroperoxy ring decomposition
C3H5O#3OOH=>R2OH+HCHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DHC 2086
C3H5O#4OOH=>R2OH+HCHO+R13CH2CHO    7.0E+14  0.0  42000.0  ! DHC 2087
C4H7O#3OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2088
C4H7O#4OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2089
C4H7O#5OOH=>R2OH+HCHO+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2090
C7H13O#3OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2091
C7H13O#4OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2092
C7H13O#5OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2093
C7H13O#6OOH=>R2OH+HCHO+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2094
C8H15O#4OOH=>R2OH+HCHO+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2095
C8H15O#5OOH=>R2OH+HCHO+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2096
C8H15O#6OOH=>R2OH+HCHO+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2097
C8H15O#3OOH=>R2OH+HCHO+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2098
C5H9O#3OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2099
C5H9O#4OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2100
C5H9O#5OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2101
C5H9O#6OOH=>R2OH+HCHO+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! DHC 2102

! Alcane reactions
C3H8+R1H=>H2+R4CH3+C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2103
C3H8+R2OH=>H2O+R4CH3+C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2104
C3H8+R3O2H=>H2O2+R4CH3+C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2105
C3H8+R4CH3=>CH4+R4CH3+C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2106
C3H8+R11C2H5=>C2H6+R4CH3+C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2107
C4H10+R1H=>H2+R11C2H5+C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2108
C4H10+R2OH=>H2O+R11C2H5+C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2109
C4H10+R3O2H=>H2O2+R11C2H5+C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2110
C4H10+R4CH3=>CH4+R11C2H5+C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2111
C4H10+R11C2H5=>C2H6+R11C2H5+C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2112
C5H12+R1H=>H2+R4CH3+2C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2113
C5H12+R2OH=>H2O+R4CH3+2C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2114
C5H12+R3O2H=>H2O2+R4CH3+2C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2115
C5H12+R4CH3=>CH4+R4CH3+2C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2116
C5H12+R11C2H5=>C2H6+R4CH3+2C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2117
C6H14+R1H=>H2+R11C2H5+2C2H4Z    2.7E+07  2.0  5000.0  ! ALC 2118
C6H14+R2OH=>H2O+R11C2H5+2C2H4Z    7.8E+06  2.0  -765.0  ! ALC 2119
C6H14+R3O2H=>H2O2+R11C2H5+2C2H4Z    1.2E+12  0.0  15500.0  ! ALC 2120
C6H14+R4CH3=>CH4+R11C2H5+2C2H4Z    6.0E+11  0.0  9600.0  ! ALC 2121
C6H14+R11C2H5=>C2H6+R11C2H5+2C2H4Z    6.0E+11  0.0  11000.0  ! ALC 2122

! O-ring decomposition

C3H6O#3+R1H=>H2+CH2COZ+R4CH3    2.7E+07  2.0  5000.0  ! ??? 2123
C3H6O#3+R2OH=>H2O+CH2COZ+R4CH3    7.8E+06  2.0  -765.0  ! ??? 2124
C3H6O#3+R3O2H=>H2O2+CH2COZ+R4CH3    1.2E+12  0.0  15500.0  ! ??? 2125
C3H6O#3+R4CH3=>CH4+CH2COZ+R4CH3    6.0E+11  0.0  9600.0  ! ??? 2126
C3H6O#3+R11C2H5=>C2H6+CH2COZ+R4CH3    6.0E+11  0.0  11000.0  ! ??? 2127
C4H8O#3+R1H=>H2+CH2COZ+R11C2H5    2.7E+07  2.0  5000.0  ! ??? 2128
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C4H8O#3+R2OH=>H2O+CH2COZ+R11C2H5    7.8E+06  2.0  -765.0  ! ??? 2129
C4H8O#3+R3O2H=>H2O2+CH2COZ+R11C2H5    1.2E+12  0.0  15500.0  ! ??? 2130
C4H8O#3+R4CH3=>CH4+CH2COZ+R11C2H5    6.0E+11  0.0  9600.0  ! ??? 2131
C4H8O#3+R11C2H5=>C2H6+CH2COZ+R11C2H5    6.0E+11  0.0  11000.0  ! ??? 2132
C7H14O#3+R1H=>H2+CH2COZ+R4CH3+2C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2133
C7H14O#3+R2OH=>H2O+CH2COZ+R4CH3+2C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2134
C7H14O#3+R3O2H=>H2O2+CH2COZ+R4CH3+2C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2135
C7H14O#3+R4CH3=>CH4+CH2COZ+R4CH3+2C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2136
C7H14O#3+R11C2H5=>C2H6+CH2COZ+R4CH3+2C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2137
C8H16O#3+R1H=>H2+CH2COZ+R11C2H5+2C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2138
C8H16O#3+R2OH=>H2O+CH2COZ+R11C2H5+2C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2139
C8H16O#3+R3O2H=>H2O2+CH2COZ+R11C2H5+2C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2140
C8H16O#3+R4CH3=>CH4+CH2COZ+R11C2H5+2C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2141
C8H16O#3+R11C2H5=>C2H6+CH2COZ+R11C2H5+2C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2142
C5H10O#3+R1H=>H2+CH2COZ+R4CH3+C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2143
C5H10O#3+R2OH=>H2O+CH2COZ+R4CH3+C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2144
C5H10O#3+R3O2H=>H2O2+CH2COZ+R4CH3+C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2145
C5H10O#3+R4CH3=>CH4+CH2COZ+R4CH3+C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2146
C5H10O#3+R11C2H5=>C2H6+CH2COZ+R4CH3+C2H4Z    6.0E+11  0.0  11000.0  ! ??? 2147
C4H#3OH10COYCOOH+R1H=>H2+CH2COZ+R11C2H5+C2H4Z    2.7E+07  2.0  5000.0  ! ??? 2148
C4H#3OH10COYCOOH+R2OH=>H2O+CH2COZ+R11C2H5+C2H4Z    7.8E+06  2.0  -765.0  ! ??? 2149
C4H#3OH10COYCOOH+R3O2H=>H2O2+CH2COZ+R11C2H5+C2H4Z    1.2E+12  0.0  15500.0  ! ??? 2150
C4H#3OH10COYCOOH+R4CH3=>CH4+CH2COZ+R11C2H5+C2H4Z    6.0E+11  0.0  9600.0  ! ??? 2151
C4H#3OH10COYCOOH+R11C2H5=>C2H6+CH2COZ+R11C2H5+C2H4Z    6.0E+11  0.0  11000.0  ! ??? 21
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! Metatheses of oxiranes and furanes
C3H6O#4+R1H=>H2+.C3H5O#4    2.7E+07  2.0  5000.0  ! ??? 2153
C3H6O#4+R2OH=>H2O+.C3H5O#4    7.8E+06  2.0  -765.0  ! ??? 2154
C3H6O#4+R3O2H=>H2O2+.C3H5O#4    1.2E+12  0.0  15500.0  ! ??? 2155
C3H6O#4+R4CH3=>CH4+.C3H5O#4    6.0E+11  0.0  9600.0  ! ??? 2156
C3H6O#4+R11C2H5=>C2H6+.C3H5O#4    6.0E+11  0.0  11000.0  ! ??? 2157
C4H8O#4+R1H=>H2+.C4H7O#4    2.7E+07  2.0  5000.0  ! ??? 2158
C4H8O#4+R2OH=>H2O+.C4H7O#4    7.8E+06  2.0  -765.0  ! ??? 2159
C4H8O#4+R3O2H=>H2O2+.C4H7O#4    1.2E+12  0.0  15500.0  ! ??? 2160
C4H8O#4+R4CH3=>CH4+.C4H7O#4    6.0E+11  0.0  9600.0  ! ??? 2161
C4H8O#4+R11C2H5=>C2H6+.C4H7O#4    6.0E+11  0.0  11000.0  ! ??? 2162
C4H8O#5+R1H=>H2+.C4H7O#5    2.7E+07  2.0  5000.0  ! ??? 2163
C4H8O#5+R2OH=>H2O+.C4H7O#5    7.8E+06  2.0  -765.0  ! ??? 2164
C4H8O#5+R3O2H=>H2O2+.C4H7O#5    1.2E+12  0.0  15500.0  ! ??? 2165
C4H8O#5+R4CH3=>CH4+.C4H7O#5    6.0E+11  0.0  9600.0  ! ??? 2166
C4H8O#5+R11C2H5=>C2H6+.C4H7O#5    6.0E+11  0.0  11000.0  ! ??? 2167
C7H14O#4+R1H=>H2+.C7H13O#4    2.7E+07  2.0  5000.0  ! DOR 1750
C7H14O#4+R2OH=>H2O+.C7H13O#4    1.9E+07  2.0  -610.0  ! DOR 1751
C7H14O#4+R3O2H=>H2O2+.C7H13O#4    1.2E+12  0.0  15500.0  ! DOR 1752
C7H14O#4+R4CH3=>CH4+.C7H13O#4    6.0E+11  0.0  9600.0  ! DOR 1753
C7H14O#4+R11C2H5=>C2H6+.C7H13O#4    6.0E+11  0.0  11000.0  ! DOR 1754
C7H14O#5+R1H=>H2+.C7H13O#5    2.7E+07  2.0  5000.0  ! DOR 1755
C7H14O#5+R2OH=>H2O+.C7H13O#5    1.4E+07  2.0  -1370.0  ! DOR 1756
C7H14O#5+R3O2H=>H2O2+.C7H13O#5    1.2E+12  0.0  15500.0  ! DOR 1757
C7H14O#5+R4CH3=>CH4+.C7H13O#5    6.0E+11  0.0  9600.0  ! DOR 1758
C7H14O#5+R11C2H5=>C2H6+.C7H13O#5    6.0E+11  0.0  11000.0  ! DOR 1759
C7H14O#6+R1H=>H2+.C7H13O#6    2.7E+07  2.0  5000.0  ! DOR 1755
C7H14O#6+R2OH=>H2O+.C7H13O#6    1.4E+07  2.0  -1370.0  ! DOR 1756
C7H14O#6+R3O2H=>H2O2+.C7H13O#6    1.2E+12  0.0  15500.0  ! DOR 1757
C7H14O#6+R4CH3=>CH4+.C7H13O#6    6.0E+11  0.0  9600.0  ! DOR 1758
C7H14O#6+R11C2H5=>C2H6+.C7H13O#6    6.0E+11  0.0  11000.0  ! DOR 1759
C8H16O#4+R1H=>H2+.C8H15O#4    2.7E+07  2.0  5000.0  ! ??? 2183
C8H16O#4+R2OH=>H2O+.C8H15O#4    7.8E+06  2.0  -765.0  ! ??? 2184
C8H16O#4+R3O2H=>H2O2+.C8H15O#4    1.2E+12  0.0  15500.0  ! ??? 2185
C8H16O#4+R4CH3=>CH4+.C8H15O#4    6.0E+11  0.0  9600.0  ! ??? 2186
C8H16O#4+R11C2H5=>C2H6+.C8H15O#4    6.0E+11  0.0  11000.0  ! ??? 2187
C8H16O#5+R1H=>H2+.C8H15O#5    2.7E+07  2.0  5000.0  ! ??? 2188
C8H16O#5+R2OH=>H2O+.C8H15O#5    7.8E+06  2.0  -765.0  ! ??? 2189
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C8H16O#5+R3O2H=>H2O2+.C8H15O#5    1.2E+12  0.0  15500.0  ! ??? 2190
C8H16O#5+R4CH3=>CH4+.C8H15O#5    6.0E+11  0.0  9600.0  ! ??? 2191
C8H16O#5+R11C2H5=>C2H6+.C8H15O#5    6.0E+11  0.0  11000.0  ! ??? 2192
C8H16O#6+R1H=>H2+.C8H15O#6    2.7E+07  2.0  5000.0  ! ??? 2193
C8H16O#6+R2OH=>H2O+.C8H15O#6    7.8E+06  2.0  -765.0  ! ??? 2194
C8H16O#6+R3O2H=>H2O2+.C8H15O#6    1.2E+12  0.0  15500.0  ! ??? 2195
C8H16O#6+R4CH3=>CH4+.C8H15O#6    6.0E+11  0.0  9600.0  ! ??? 2196
C8H16O#6+R11C2H5=>C2H6+.C8H15O#6    6.0E+11  0.0  11000.0  ! ??? 2197
C5H10O#4+R1H=>H2+.C5H9O#4    2.7E+07  2.0  5000.0  ! ??? 2198
C5H10O#4+R2OH=>H2O+.C5H9O#4    7.8E+06  2.0  -765.0  ! ??? 2199
C5H10O#4+R3O2H=>H2O2+.C5H9O#4    1.2E+12  0.0  15500.0  ! ??? 2200
C5H10O#4+R4CH3=>CH4+.C5H9O#4    6.0E+11  0.0  9600.0  ! ??? 2201
C5H10O#4+R11C2H5=>C2H6+.C5H9O#4    6.0E+11  0.0  11000.0  ! ??? 2202
C5H10O#5+R1H=>H2+.C5H9O#5    2.7E+07  2.0  5000.0  ! ??? 2203
C5H10O#5+R2OH=>H2O+.C5H9O#5    7.8E+06  2.0  -765.0  ! ??? 2204
C5H10O#5+R3O2H=>H2O2+.C5H9O#5    1.2E+12  0.0  15500.0  ! ??? 2205
C5H10O#5+R4CH3=>CH4+.C5H9O#5    6.0E+11  0.0  9600.0  ! ??? 2206
C5H10O#5+R11C2H5=>C2H6+.C5H9O#5    6.0E+11  0.0  11000.0  ! ??? 2207
C5H10O#6+R1H=>H2+.C5H9O#6    2.7E+07  2.0  5000.0  ! ??? 2208
C5H10O#6+R2OH=>H2O+.C5H9O#6    7.8E+06  2.0  -765.0  ! ??? 2209
C5H10O#6+R3O2H=>H2O2+.C5H9O#6    1.2E+12  0.0  15500.0  ! ??? 2210
C5H10O#6+R4CH3=>CH4+.C5H9O#6    6.0E+11  0.0  9600.0  ! ??? 2211
C5H10O#6+R11C2H5=>C2H6+.C5H9O#6    6.0E+11  0.0  11000.0  ! ??? 2212

! decompositions of cyclo-ether radicals
.C3H5O#4=>R5CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2213
.C4H7O#4=>R13CH2CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2214
.C4H7O#5=>R13CH2CHO+C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2215
.C7H13O#4=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2216
.C7H13O#5=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2217
.C7H13O#6=>R5CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2218
.C8H15O#4=>R13CH2CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2219
.C8H15O#5=>R13CH2CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2220
.C8H15O#6=>R13CH2CHO+3C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2221
.C5H9O#4=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2222
.C5H9O#5=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2223
.C5H9O#6=>R5CHO+2C2H4Z    5.0E+13  0.0  24800.0  ! ??? 2224

! Addition of oxygen on cyclo-ether radicals
.C3H5O#4+O2=>.OOC3H5O#4    2.2E+19  -2.5  0.0  ! ??? 2225
.C4H7O#4+O2=>.OOC4H7O#4    2.2E+19  -2.5  0.0  ! ??? 2226
.C4H7O#5+O2=>.OOC4H7O#5    2.2E+19  -2.5  0.0  ! ??? 2227
.C7H13O#4+O2=>.OOC7H13O#4    2.2E+19  -2.5  0.0  ! ??? 2228
.C7H13O#5+O2=>.OOC7H13O#5    2.2E+19  -2.5  0.0  ! ??? 2229
.C7H13O#6+O2=>.OOC7H13O#6    2.2E+19  -2.5  0.0  ! ??? 2230
.C8H15O#4+O2=>.OOC8H15O#4    2.2E+19  -2.5  0.0  ! ??? 2231
.C8H15O#5+O2=>.OOC8H15O#5    2.2E+19  -2.5  0.0  ! ??? 2232
.C8H15O#6+O2=>.OOC8H15O#6    2.2E+19  -2.5  0.0  ! ??? 2233
.C5H9O#4+O2=>.OOC5H9O#4    2.2E+19  -2.5  0.0  ! ??? 2234
.C5H9O#5+O2=>.OOC5H9O#5    2.2E+19  -2.5  0.0  ! ??? 2235
.C5H9O#6+O2=>.OOC5H9O#6    2.2E+19  -2.5  0.0  ! ??? 2236
.OOC3H5O#4=>.C3H5O#4 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2237
.OOC4H7O#4=>.C4H7O#4 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2238
.OOC4H7O#5=>.C4H7O#5 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2239
.OOC7H13O#4=>.C7H13O#4 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2240
.OOC7H13O#5=>.C7H13O#5 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2241
.OOC7H13O#6=>.C7H13O#6 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2242
.OOC8H15O#4=>.C8H15O#4 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2243
.OOC8H15O#5=>.C8H15O#5 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2244
.OOC8H15O#6=>.C8H15O#6 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2245
.OOC5H9O#4=>.C5H9O#4 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2246
.OOC5H9O#5=>.C5H9O#5 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2247
.OOC5H9O#6=>.C5H9O#6 +  O2    5.0E+22  -2.5  36000.0  ! ??? 2248
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! Isomerization of peroxy-radicals
.OOC3H5O#4=>.C3H4O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2249
.OOC4H7O#4=>.C4H6O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2250
.OOC4H7O#5=>.C4H6O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2251
.OOC7H13O#4=>.C7H12O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2252
.OOC7H13O#5=>.C7H12O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2253
.OOC7H13O#6=>.C7H12O#6OOH    8.0E+13  0.0  25500.0  ! ??? 2254
.OOC8H15O#4=>.C8H14O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2255
.OOC8H15O#5=>.C8H14O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2256
.OOC8H15O#6=>.C8H14O#6OOH    8.0E+13  0.0  25500.0  ! ??? 2257
.OOC5H9O#4=>.C5H8O#4OOH    8.0E+13  0.0  25500.0  ! ??? 2258
.OOC5H9O#5=>.C5H8O#5OOH    8.0E+13  0.0  25500.0  ! ??? 2259
.OOC5H9O#6=>.C5H8O#6OOH    8.0E+13  0.0  25500.0  ! ??? 2260
.C3H4O#4OOH=>.OOC3H5O#4    4.8E+12  0.0  19000.0  ! ??? 2261
.C4H6O#4OOH=>.OOC4H7O#4    4.8E+12  0.0  19000.0  ! ??? 2262
.C4H6O#5OOH=>.OOC4H7O#5    4.8E+12  0.0  19000.0  ! ??? 2263
.C7H12O#4OOH=>.OOC7H13O#4    4.8E+12  0.0  19000.0  ! ??? 2264
.C7H12O#5OOH=>.OOC7H13O#5    4.8E+12  0.0  19000.0  ! ??? 2265
.C7H12O#6OOH=>.OOC7H13O#6    4.8E+12  0.0  19000.0  ! ??? 2266
.C8H14O#4OOH=>.OOC8H15O#4    4.8E+12  0.0  19000.0  ! ??? 2267
.C8H14O#5OOH=>.OOC8H15O#5    4.8E+12  0.0  19000.0  ! ??? 2268
.C8H14O#6OOH=>.OOC8H15O#6    4.8E+12  0.0  19000.0  ! ??? 2269
.C5H8O#4OOH=>.OOC5H9O#4    4.8E+12  0.0  19000.0  ! ??? 2270
.C5H8O#5OOH=>.OOC5H9O#5    4.8E+12  0.0  19000.0  ! ??? 2271
.C5H8O#6OOH=>.OOC5H9O#6    4.8E+12  0.0  19000.0  ! ??? 2272

!Addition of oxygen on cyclo-peroxy radicals
.C3H4O#4OOH+O2=>.OOC3H4O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2273
.C4H6O#4OOH+O2=>.OOC4H6O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2274
.C4H6O#5OOH+O2=>.OOC4H6O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2275
.C7H12O#4OOH+O2=>.OOC7H12O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2276
.C7H12O#5OOH+O2=>.OOC7H12O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2277
.C7H12O#6OOH+O2=>.OOC7H12O#6OOH    2.2E+19  -2.5  0.0  ! ??? 2278
.C8H14O#4OOH+O2=>.OOC8H14O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2279
.C8H14O#5OOH+O2=>.OOC8H14O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2280
.C8H14O#6OOH+O2=>.OOC8H14O#6OOH    2.2E+19  -2.5  0.0  ! ??? 2281
.C5H8O#4OOH+O2=>.OOC5H8O#4OOH    2.2E+19  -2.5  0.0  ! ??? 2282
.C5H8O#5OOH+O2=>.OOC5H8O#5OOH    2.2E+19  -2.5  0.0  ! ??? 2283
.C5H8O#6OOH+O2=>.OOC5H8O#6OOH    2.2E+19  -2.5  0.0  ! ??? 2284
.OOC3H4O#4OOH=>.C3H4O#4OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2285
.OOC4H6O#4OOH=>.C4H6O#4OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2286
.OOC4H6O#5OOH=>.C4H6O#5OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2287
.OOC7H12O#4OOH=>.C7H12O#4OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2288
.OOC7H12O#5OOH=>.C7H12O#5OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2289
.OOC7H12O#6OOH=>.C7H12O#6OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2290
.OOC8H14O#4OOH=>.C8H14O#4OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2291
.OOC8H14O#5OOH=>.C8H14O#5OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2292
.OOC8H14O#6OOH=>.C8H14O#6OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2293
.OOC5H8O#4OOH=>.C5H8O#4OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2294
.OOC5H8O#5OOH=>.C5H8O#5OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2295
.OOC5H8O#6OOH=>.C5H8O#6OOH +  O2    5.0E+22  -2.5  36000.0  ! ??? 2296

! Formation of cyclo-ether ketohydroperoxydes
.OOC3H4O#4OOH=>R2OH+C2H3O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2297
.OOC4H6O#4OOH=>R2OH+C3H5O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2298
.OOC4H6O#5OOH=>R2OH+C3H5O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2299
.OOC7H12O#4OOH=>R2OH+C6H11O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2300
.OOC7H12O#5OOH=>R2OH+C6H11O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2301
.OOC7H12O#6OOH=>R2OH+C6H11O#6COOOH    1.0E+09  0.0  7500.0  ! ??? 2302
.OOC8H14O#4OOH=>R2OH+C7H13O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2303
.OOC8H14O#5OOH=>R2OH+C7H13O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2304
.OOC8H14O#6OOH=>R2OH+C7H13O#6COOOH    1.0E+09  0.0  7500.0  ! ??? 2305
.OOC5H8O#4OOH=>R2OH+C4H7O#4COOOH    1.0E+09  0.0  7500.0  ! ??? 2306
.OOC5H8O#5OOH=>R2OH+C4H7O#5COOOH    1.0E+09  0.0  7500.0  ! ??? 2307
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.OOC5H8O#6OOH=>R2OH+C4H7O#6COOOH    1.0E+09  0.0  7500.0  ! ??? 2308

! Decomposition of cyclo-ether ketohydroperoxydes
C2H3O#4COOOH=>R2OH+CO2+R13CH2CHO    7.0E+14  0.0  42000.0  ! ??? 2309
C3H5O#4COOOH=>R2OH+CO2+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2310
C3H5O#5COOOH=>R2OH+CO2+R5CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2311
C6H11O#4COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2312
C6H11O#5COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2313
C6H11O#6COOOH=>R2OH+CO2+R13CH2CHO+2C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2314
C7H13O#4COOOH=>R2OH+CO2+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2315
C7H13O#5COOOH=>R2OH+CO2+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2316
C7H13O#6COOOH=>R2OH+CO2+R5CHO+3C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2317
C4H7O#4COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2318
C4H7O#5COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2319
C4H7O#6COOOH=>R2OH+CO2+R13CH2CHO+C2H4Z    7.0E+14  0.0  42000.0  ! ??? 2320

! Olefin reactions to product products of the base
C3H6Y+R1H=>C2H4Z+R4CH3        7.2E+12  0.0  2900.0  ! ROL 206
C3H6Y+R4CH3=>C2H4Z+R11C2H5    9.6E+10  0.0  8000.0  ! ROL 207
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
C7H14Y+R1H=>3C2H4Z+R4CH3             7.2E+12  0.0  2900.0  ! ROL 210
C7H14Y+R1H=>C3H6Y+R11C2H5+C2H4Z      7.2E+12  0.0  1300.0  ! ROL 210'
C7H14Y+R4CH3=>C3H6Y+R4CH3+2C2H4Z     9.6E+10  0.0  8000.0  ! ROL 211
C7H14Y+R4CH3=>C4H8Y+R11C2H5+C2H4Z    1.7E+11  0.0  7400.0  ! ROL 211
C5H10Y+R1H=>2C2H4Z+R4CH3             7.2E+12  0.0  2900.0  ! ROL 218
C5H10Y+R1H=>C3H6Y+R11C2H5            7.2E+12  0.0  1300.0  ! ROL 218'
C5H10Y+R4CH3=>C3H6Y+R4CH3+C2H4Z      9.6E+10  0.0  8000.0  ! ROL 219
C5H10Y+R4CH3=>C4H8Y+R11C2H5          1.7E+11  0.0  7400.0  ! ROL 219
C8H16Y+R1H=>3C2H4Z+R11C2H5           7.2E+12  0.0  2900.0
C8H16Y+R1H=>C3H6Y+R4CH3+2C2H4Z       7.2E+12  0.0  1300.0
C8H16Y+R4CH3=>4C2H4Z+R4CH3           9.6E+10  0.0  8000.0
C8H16Y+R4CH3=>C4H8Y+R4CH3+2C2H4Z     1.7E+11  0.0  7400.0  ! ROL 217
C6H12Z+R1H=>2C2H4Z+R11C2H5           7.2E+12  0.0  2900.0  ! ROL 2329
C6H12Z+R1H=>C3H6Y+R4CH3+C2H4Z        7.2E+12  0.0  1300.0  ! ROL 2329
C6H12Z+R4CH3=>3C2H4Z+R4CH3           9.6E+10  0.0  8000.0  ! ROL 2330
C6H12Z+R4CH3=>C4H8Y+R4CH3+C2H4Z      1.7E+11  0.0  7400.0  ! ROL 217


!  olefin to aldehydes
C3H6Y+R2OH=>R4CH3+CH3CHO    2.9E+12  0.0  -900.0  ! ALD 179
C4H8Y+R2OH=>R4CH3+C2H5CHO    1.4E+12  0.0  -900.0  ! ALD 180
C7H14Y+R2OH=>R4CH3+C5H11CHO    1.4E+12  0.0  -900.0  ! ALD 181
C8H16Y+R2OH=>R4CH3+C6H13CHO    1.4E+12  0.0  -900.0  ! ALD 182
C5H10Y+R2OH=>R4CH3+C3H7CHO    1.4E+12  0.0  -900.0  ! ALD 184
C6H12Z+R2OH=>R4CH3+C4H9CHO    2.0E+00  4.0  -1000.0  ! ALD 2337


!  olefin to alkohols remplace par :
C4H8Y+R2OH=>HCHO+C2H4Z+R4CH3    1.4E+12  0.0  -900.0  ! FOH 185
C7H14Y+R2OH=>HCHO+2C2H4Z+R11C2H5    1.4E+12  0.0  -900.0  ! FOH 186
C8H16Y+R2OH=>HCHO+3C2H4Z+R4CH3    1.4E+12  0.0  -900.0  ! FOH 187
C6H12Z+R2OH=>HCHO+2C2H4Z+R4CH3    1.4E+12  0.0  -900.0  ! FOH 2342
C5H10Y+R2OH=>HCHO+C2H4Z+R11C2H5    1.4E+12  0.0  -900.0  ! FOH 189
C3H6Y+R2OH=>HCHO+R11C2H5    1.4E+12  0.0  -900.0  ! FOH 189


!   olefin to dienes
C6H12Z+R1H=>H2+R11C2H5+C4H6Z2    8.9E+06  2.0  3000.0  ! FZZ 2354
C6H12Z+R2OH=>H2O+R11C2H5+C4H6Z2    2.57E+06  2.0  -2700.0  ! FZZ 2355
C6H12Z+R3O2H=>H2O2+R11C2H5+C4H6Z2    4.0E+11  0.0  13500.0  ! FZZ 2356
C6H12Z+R4CH3=>CH4+R11C2H5+C4H6Z2    2.0E+11  0.0  7500.0  ! FZZ 2357
C6H12Z+R11C2H5=>C2H6+R11C2H5+C4H6Z2    2.0E+11  0.0  9000.0  ! FZZ 2358
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!   addition de O sur les alcenes lourds                                    *****
C4H8Y+B1O=>R1H+CH2COZ+R11C2H5   3.4E+07  1.83   -550.0
C3H6Y+B1O=>R1H+CH2COZ+R4CH3   3.4E+07  1.83   -550.0
C5H10Y+B1O=>R1H+CH2COZ+R4CH3+C2H4Z    3.4E+07  1.83   -550.0
C6H12Z+B1O=>R1H+CH2COZ+R11C2H5+C2H4Z   3.4E+07  1.83   -550.0
C7H14Y+B1O=>R1H+CH2COZ+R4CH3+2C2H4Z   3.4E+07  1.83   -550.0
C8H16Y+B1O=>R1H+CH2COZ+R11C2H5+2C2H4Z   3.4E+07  1.83   -550.0


!  epoxy formation
C3H6Y+R3O2H=>R2OH+C3H6O#3    1.0E+12  0.0  14400.0  ! FCY 2364
C4H8Y+R3O2H=>R2OH+C4H8O#3    1.0E+12  0.0  14400.0  ! FCY 2365
C5H10Y+R3O2H=>R2OH+C5H10O#3    1.0E+12  0.0  14400.0  ! FCY 2366
C7H14Y+R3O2H=>R2OH+C7H14O#3    1.0E+12  0.0  14400.0  ! FCY 2367
C6H12Z+R3O2H=>R2OH+C4H#3OH10COYCOOH    1.0E+12  0.0  14400.0  ! FCY 2368
C8H16Y+R3O2H=>R2OH+C8H16O#3    1.0E+12  0.0  14400.0  ! FCY 2369

! Alkohol reactions
C3H7OH+R1H=>H2+R2OH+C3H6Y    9.0E+06  2.0  5000.0  ! AL 2370
C3H7OH+R1H=>H2+R4CH3+CH3CHO    4.2E+06  2.0  2400.0  ! AL 2371
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    1.3E+09  1.3  700.0  ! AL 2372
C3H7OH+R2OH=>H2O+R4CH3+CH3CHO    4.0E+12  0.0  443.0  ! AL 2373
C3H7OH+R3O2H=>H2O2+R2OH+C3H6Y    4.0E+11  0.0  15500.0  ! AL 2374
C3H7OH+R3O2H=>H2O2+R4CH3+CH3CHO    1.0E+12  0.0  14000.0  ! AL 2375
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    2.0E+11  0.0  9600.0  ! AL 2376
C3H7OH+R4CH3=>CH4+R4CH3+CH3CHO    1.0E+11  0.0  7600.0  ! AL 2377
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    2.0E+11  0.0  11000.0  ! AL 2378
C3H7OH+R11C2H5=>C2H6+R4CH3+CH3CHO    1.0E+11  0.0  9200.0  ! AL 2379
C4H9OH+R1H=>H2+R2OH+C4H8Y    9.0E+06  2.0  5000.0  ! AL 2380
C4H9OH+R1H=>H2+R4CH3+C2H5CHO    4.2E+06  2.0  2400.0  ! AL 2381
C4H9OH+R1H=>H2+R4CH3+C2H6CO    4.2E+06  2.0  2400.0  ! AL 2382
C4H9OH+R2OH=>H2O+R2OH+C4H8Y    1.3E+09  1.3  700.0  ! AL 2383
C4H9OH+R2OH=>H2O+R4CH3+C2H5CHO    4.0E+12  0.0  443.0  ! AL 2384
C4H9OH+R2OH=>H2O+R4CH3+C2H6CO    4.0E+12  0.0  443.0  ! AL 2385
C4H9OH+R3O2H=>H2O2+R2OH+C4H8Y    4.0E+11  0.0  15500.0  ! AL 2386
C4H9OH+R3O2H=>H2O2+R4CH3+C2H5CHO    1.0E+12  0.0  14000.0  ! AL 2387
C4H9OH+R3O2H=>H2O2+R4CH3+C2H6CO    1.0E+12  0.0  14000.0  ! AL 2388
C4H9OH+R4CH3=>CH4+R2OH+C4H8Y    2.0E+11  0.0  9600.0  ! AL 2389
C4H9OH+R4CH3=>CH4+R4CH3+C2H5CHO    1.0E+11  0.0  7600.0  ! AL 2390
C4H9OH+R4CH3=>CH4+R4CH3+C2H6CO    1.0E+11  0.0  7600.0  ! AL 2391
C4H9OH+R11C2H5=>C2H6+R2OH+C4H8Y    2.0E+11  0.0  11000.0  ! AL 2392
C4H9OH+R11C2H5=>C2H6+R4CH3+C2H5CHO    1.0E+11  0.0  9200.0  ! AL 2393
C4H9OH+R11C2H5=>C2H6+R4CH3+C2H6CO    1.0E+11  0.0  9200.0  ! AL 2394
C5H11OH+R1H=>H2+R2OH+C5H10Y    9.0E+06  2.0  5000.0  ! AL 2395
C5H11OH+R1H=>H2+R4CH3+C3H7CHO    4.2E+06  2.0  2400.0  ! AL 2396
C5H11OH+R1H=>H2+R4CH3+C3H8CO    4.2E+06  2.0  2400.0  ! AL 2397
C5H11OH+R2OH=>H2O+R2OH+C5H10Y    1.3E+09  1.3  700.0  ! AL 2398
C5H11OH+R2OH=>H2O+R4CH3+C3H7CHO    4.0E+12  0.0  443.0  ! AL 2399
C5H11OH+R2OH=>H2O+R4CH3+C3H8CO    4.0E+12  0.0  443.0  ! AL 2400
C5H11OH+R3O2H=>H2O2+R2OH+C5H10Y    4.0E+11  0.0  15500.0  ! AL 2401
C5H11OH+R3O2H=>H2O2+R4CH3+C3H7CHO    1.0E+12  0.0  14000.0  ! AL 2402
C5H11OH+R3O2H=>H2O2+R4CH3+C3H8CO    1.0E+12  0.0  14000.0  ! AL 2403
C5H11OH+R4CH3=>CH4+R2OH+C5H10Y    2.0E+11  0.0  9600.0  ! AL 2404
C5H11OH+R4CH3=>CH4+R4CH3+C3H7CHO    1.0E+11  0.0  7600.0  ! AL 2405
C5H11OH+R4CH3=>CH4+R4CH3+C3H8CO    1.0E+11  0.0  7600.0  ! AL 2406
C5H11OH+R11C2H5=>C2H6+R2OH+C5H10Y    2.0E+11  0.0  11000.0  ! AL 2407
C5H11OH+R11C2H5=>C2H6+R4CH3+C3H7CHO    1.0E+11  0.0  9200.0  ! AL 2408
C5H11OH+R11C2H5=>C2H6+R4CH3+C3H8CO    1.0E+11  0.0  9200.0  ! AL 2409

! Metathesis with YH
C3H6Y+R1H=>.C3H5Y+H2    1.7E+05  2.5  2490.0  ! MES 2410
C3H6Y+R2OH=>.C3H5Y+H2O    3.1E+06  2.0  -300.0  ! MES 2411
C3H6Y+R3O2H=>.C3H5Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2412
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C3H6Y+R4CH3=>.C3H5Y+CH4    2.2E+00  3.5  5675.0  ! MES 2413
C3H6Y+R11C2H5=>.C3H5Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2414
C4H8Y+R1H=>.C4H7Y+H2    1.7E+05  2.5  2490.0  ! MES 2415
C4H8Y+R2OH=>.C4H7Y+H2O    3.1E+06  2.0  -300.0  ! MES 2416
C4H8Y+R3O2H=>.C4H7Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2417
C4H8Y+R4CH3=>.C4H7Y+CH4    2.2E+00  3.5  5675.0  ! MES 2418
C4H8Y+R11C2H5=>.C4H7Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2419
C5H10Y+R1H=>.C5H9Y+H2    1.7E+05  2.5  2490.0  ! MES 2420
C5H10Y+R2OH=>.C5H9Y+H2O    3.1E+06  2.0  -300.0  ! MES 2421
C5H10Y+R3O2H=>.C5H9Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2422
C5H10Y+R4CH3=>.C5H9Y+CH4    2.2E+00  3.5  5675.0  ! MES 2423
C5H10Y+R11C2H5=>.C5H9Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2424
C7H14Y+R1H=>.C7H13Y+H2    1.7E+05  2.5  2490.0  ! MES 2425
C7H14Y+R2OH=>.C7H13Y+H2O    3.1E+06  2.0  -300.0  ! MES 2426
C7H14Y+R3O2H=>.C7H13Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2427
C7H14Y+R4CH3=>.C7H13Y+CH4    2.2E+00  3.5  5675.0  ! MES 2428
C7H14Y+R11C2H5=>.C7H13Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2429
C8H16Y+R1H=>.C8H15Y+H2    1.7E+05  2.5  2490.0  ! MES 2430
C8H16Y+R2OH=>.C8H15Y+H2O    3.1E+06  2.0  -300.0  ! MES 2431
C8H16Y+R3O2H=>.C8H15Y+H2O2    9.6E+03  2.6  13900.0  ! MES 2432
C8H16Y+R4CH3=>.C8H15Y+CH4    2.2E+00  3.5  5675.0  ! MES 2433
C8H16Y+R11C2H5=>.C8H15Y+C2H6    2.2E+00  3.5  6835.0  ! MES 2434
C3H6Y+B1O=>.C3H5Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2435
C4H8Y+B1O=>.C4H7Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2436
C5H10Y+B1O=>.C5H9Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2437
C7H14Y+B1O=>.C7H13Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2438
C8H16Y+B1O=>.C8H15Y+R2OH    6.0E+10  0.7  7682.0  ! MES 2439

! Addition of .Y on YH
.C3H5Y+C8H16Y=>R4CH3+C2H2+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2440
.C3H5Y+C7H14Y=>R10C2H3V+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2441
.C3H5Y+C5H10Y=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2442
.C3H5Y+C4H8Y=>R4CH3+C2H2+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2443
.C3H5Y+C3H6Y=>R10C2H3V+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2444
.C4H7Y+C8H16Y=>R10C2H3V+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2445
.C4H7Y+C7H14Y=>R4CH3+C2H2+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2446
.C4H7Y+C5H10Y=>R4CH3+C2H2+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2447
.C4H7Y+C4H8Y=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2448
.C4H7Y+C3H6Y=>R4CH3+C2H2+2C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2449
.C5H9Y+C8H16Y=>R4CH3+C2H2+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2450
.C5H9Y+C7H14Y=>R10C2H3V+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2451
.C5H9Y+C5H10Y=>R10C2H3V+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2452
.C5H9Y+C4H8Y=>R4CH3+C2H2+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2453
.C5H9Y+C3H6Y=>R10C2H3V+3C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2454
.C7H13Y+C8H16Y=>R4CH3+C2H2+6C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2455
.C7H13Y+C7H14Y=>R10C2H3V+6C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2456
.C7H13Y+C5H10Y=>R10C2H3V+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2457
.C7H13Y+C4H8Y=>R4CH3+C2H2+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2458
.C7H13Y+C3H6Y=>R10C2H3V+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2459
.C8H15Y+C8H16Y=>R10C2H3V+7C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2460
.C8H15Y+C7H14Y=>R4CH3+C2H2+6C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2461
.C8H15Y+C5H10Y=>R4CH3+C2H2+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2462
.C8H15Y+C4H8Y=>R10C2H3V+5C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2463
.C8H15Y+C3H6Y=>R4CH3+C2H2+4C2H4Z    6.0E+09  0.0  11400.0  ! ADY 2464

! Aldehydes metathesis
C2H5CHO+R1H=>H2+.COC2H5    4.0E+13  0.0  4200.0  ! ALD 2465
C2H5CHO+R2OH=>H2O+.COC2H5    4.2E+12  0.0  500.0  ! ALD 2466
C2H5CHO+R4CH3=>CH4+.COC2H5    2.0E-06  5.6  2500.0  ! ALD 2467
C2H5CHO+R11C2H5=>C2H6+.COC2H5    1.3E+12  0.0  8500.0  ! ALD 2468
C3H7CHO+R1H=>H2+.COC3H7    4.0E+13  0.0  4200.0  ! ALD 2469
C3H7CHO+R2OH=>H2O+.COC3H7    4.2E+12  0.0  500.0  ! ALD 2470
C3H7CHO+R4CH3=>CH4+.COC3H7    2.0E-06  5.6  2500.0  ! ALD 2471
C3H7CHO+R11C2H5=>C2H6+.COC3H7    1.3E+12  0.0  8500.0  ! ALD 2472
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C4H9CHO+R1H=>H2+.COC4H9    4.0E+13  0.0  4200.0  ! ALD 2473
C4H9CHO+R2OH=>H2O+.COC4H9    4.2E+12  0.0  500.0  ! ALD 2474
C4H9CHO+R4CH3=>CH4+.COC4H9    2.0E-06  5.6  2500.0  ! ALD 2475
C4H9CHO+R11C2H5=>C2H6+.COC4H9    1.3E+12  0.0  8500.0  ! ALD 2476
C6H13CHO+R1H=>H2+.COC6H13    4.0E+13  0.0  4200.0  ! ALD 2477
C6H13CHO+R2OH=>H2O+.COC6H13    4.2E+12  0.0  500.0  ! ALD 2478
C6H13CHO+R4CH3=>CH4+.COC6H13    2.0E-06  5.6  2500.0  ! ALD 2479
C6H13CHO+R11C2H5=>C2H6+.COC6H13    1.3E+12  0.0  8500.0  ! ALD 2480
C7H15CHO+R1H=>H2+.COC7H15    4.0E+13  0.0  4200.0  ! ALD 2481
C7H15CHO+R2OH=>H2O+.COC7H15    4.2E+12  0.0  500.0  ! ALD 2482
C7H15CHO+R4CH3=>CH4+.COC7H15    2.0E-06  5.6  2500.0  ! ALD 2483
C7H15CHO+R11C2H5=>C2H6+.COC7H15    1.3E+12  0.0  8500.0  ! ALD 2484
C5H11CHO+R1H=>H2+.COC5H11    4.0E+13  0.0  4200.0  ! ALD 2485
C5H11CHO+R2OH=>H2O+.COC5H11    4.2E+12  0.0  500.0  ! ALD 2486
C5H11CHO+R4CH3=>CH4+.COC5H11    2.0E-06  5.6  2500.0  ! ALD 2487
C5H11CHO+R11C2H5=>C2H6+.COC5H11    1.3E+12  0.0  8500.0  ! ALD 2488

! Ketones reactions
C3H8CO+R1H=>CH3CHO+R11C2H5    7.0E+00  4.0  1300.0  ! FCO 2489
C3H8CO+R4CH3=>CH3CHO+R4CH3+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2490
C6H14CO+R1H=>C3H8CO+R4CH3+C2H4Z    7.0E+00  4.0  1300.0  ! FCO 2491
C6H14CO+R4CH3=>C3H8CO+R11C2H5+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2492
C4H10CO+R1H=>C2H6CO+R11C2H5    7.0E+00  4.0  1300.0  ! FCO 2493
C4H10CO+R4CH3=>C2H6CO+R4CH3+C2H4Z    3.0E+12  0.0  0.0  ! FCO 2494


! Acid formation
C6H14CO+R2OH=>C3H7COOH+R4CH3+C2H4Z    6.0E+11  0.0  0.0  ! FAC 2495
C4H10CO+R2OH=>C2H5COOH+R11C2H5    6.0E+11  0.0  0.0  ! FAC 2496

! Acid metathesis
C3H7COOH+R1H=>.COOC3H7+H2    4.2E+06  2.1  4900.0  ! MAC 2497
C2H5COOH+R1H=>.COOC2H5+H2    4.2E+06  2.1  4900.0  ! MAC 2498

! Ester metatesis

! Alkohol ene to dienes
C6H11OHY+R1H=>H2+R2OH+C6H10YZ    9.0E+06  2.0  5000.0  ! ROH 2499
C6H11OHY+R2OH=>H2O+R2OH+C6H10YZ    1.3E+09  1.3  700.0  ! ROH 2500
C6H11OHY+R3O2H=>H2O2+R2OH+C6H10YZ    4.0E+11  0.0  15500.0  ! ROH 2501
C6H11OHY+R4CH3=>CH4+R2OH+C6H10YZ    2.0E+11  0.0  9600.0  ! ROH 2502
C6H11OHY+R11C2H5=>C2H6+R2OH+C6H10YZ    2.0E+11  0.0  11000.0  ! ROH 2503
C5H9OHZ+R1H=>H2+R2OH+C5H8Z2    9.0E+06  2.0  5000.0  ! ROH 2504
C5H9OHZ+R2OH=>H2O+R2OH+C5H8Z2    1.3E+09  1.3  700.0  ! ROH 2505
C5H9OHZ+R3O2H=>H2O2+R2OH+C5H8Z2    4.0E+11  0.0  15500.0  ! ROH 2506
C5H9OHZ+R4CH3=>CH4+R2OH+C5H8Z2    2.0E+11  0.0  9600.0  ! ROH 2507
C5H9OHZ+R11C2H5=>C2H6+R2OH+C5H8Z2    2.0E+11  0.0  11000.0  ! ROH 2508
C7H13OHY+R1H=>H2+R2OH+C7H12YZ    9.0E+06  2.0  5000.0  ! ROH 2509
C7H13OHY+R2OH=>H2O+R2OH+C7H12YZ    1.3E+09  1.3  700.0  ! ROH 2510
C7H13OHY+R3O2H=>H2O2+R2OH+C7H12YZ    4.0E+11  0.0  15500.0  ! ROH 2511
C7H13OHY+R4CH3=>CH4+R2OH+C7H12YZ    2.0E+11  0.0  9600.0  ! ROH 2512
C7H13OHY+R11C2H5=>C2H6+R2OH+C7H12YZ    2.0E+11  0.0  11000.0  ! ROH 2513

! Diels Alder
C4H6Z2+C2H4Z=>C6H10#ZOOY    3.0E+10  0.0  27500.0  ! DA 2514
C4H6YZ+C2H4Z=>C6H10#ZOOY    3.0E+10  0.0  27500.0  ! DA 2515
C6H10YZ+C2H4Z=>C8H14#ZYZ    3.0E+10  0.0  27500.0  ! DA 2516
C5H8Z2+C2H4Z=>C7H12#ZZ2    3.0E+10  0.0  27500.0  ! DA 2517
C7H12YZ+C2H4Z=>C9H16#ZYZ    3.0E+10  0.0  27500.0  ! DA 2518

! Peracide radical metathesis
.COOOC2H5+C8H18=>R25C8H17+R2OH+CO2+R11C2H5    9.0E+12  0.0  17500.0  ! PER 2519
.COOOC2H5+C7H16=>R21C7H15+R2OH+CO2+R11C2H5    9.0E+12  0.0  17500.0  ! PER 2520
.COOOC3H7+C8H18=>R25C8H17+R2OH+CO2+R4CH3+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2521
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.COOOC3H7+C7H16=>R21C7H15+R2OH+CO2+R4CH3+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2522
.COOOC4H9+C8H18=>R25C8H17+R2OH+CO2+R11C2H5+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2523
.COOOC4H9+C7H16=>R21C7H15+R2OH+CO2+R11C2H5+C2H4Z    9.0E+12  0.0  17500.0  ! PER 2524
.COOOC6H13+C8H18=>R25C8H17+R2OH+CO2+R11C2H5+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 252
5
.COOOC6H13+C7H16=>R21C7H15+R2OH+CO2+R11C2H5+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 252
6
.COOOC7H15+C8H18=>R25C8H17+R2OH+CO2+R4CH3+3C2H4Z    9.0E+12  0.0  17500.0  ! PER 2527
.COOOC7H15+C7H16=>R21C7H15+R2OH+CO2+R4CH3+3C2H4Z    9.0E+12  0.0  17500.0  ! PER 2528
.COOOC5H11+C8H18=>R25C8H17+R2OH+CO2+R4CH3+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 2529
.COOOC5H11+C7H16=>R21C7H15+R2OH+CO2+R4CH3+2C2H4Z    9.0E+12  0.0  17500.0  ! PER 2530
.COOOC2H5=>C2H4Z+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2531
.COOOC3H7=>C3H6Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2532
.COOOC4H9=>C4H8Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2533
.COOOC6H13=>C6H12Z+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2534
.COOOC7H15=>C7H14Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2535
.COOOC5H11=>C5H10Y+R2OH+CO2    4.5E+11  0.0  25000.0  ! PER 2536

! Keto radicals to products of the base and :CO
.COC2H5=>B2CO+R11C2H5    2.0E+13  0.0  28700.0  ! COR 2537
.COC3H7=>B2CO+R4CH3+C2H4Z    2.0E+13  0.0  28700.0  ! COR 2538
.COC4H9=>B2CO+R11C2H5+C2H4Z    2.0E+13  0.0  28700.0  ! COR 2539
.COC6H13=>B2CO+R11C2H5+2C2H4Z    2.0E+13  0.0  28700.0  ! COR 2540
.COC7H15=>B2CO+R4CH3+3C2H4Z    2.0E+13  0.0  28700.0  ! COR 2541
.COC5H11=>B2CO+R4CH3+2C2H4Z    2.0E+13  0.0  28700.0  ! COR 2542


! keto radicals addition to O2
.COC2H5+O2=>.COOOC2H5    2.4E+12  0.0  0.0  ! COR 2543
.COC3H7+O2=>.COOOC3H7    2.4E+12  0.0  0.0  ! COR 2544
.COC4H9+O2=>.COOOC4H9    2.4E+12  0.0  0.0  ! COR 2545
.COC6H13+O2=>.COOOC6H13    2.4E+12  0.0  0.0  ! COR 2546
.COC7H15+O2=>.COOOC7H15    2.4E+12  0.0  0.0  ! COR 2547
.COC5H11+O2=>.COOOC5H11    2.4E+12  0.0  0.0  ! COR 2548

! Ester radicals reactions :

! .Y termination
.C3H5Y+R1H=>C3H6Y    1.0E+13  0.0  0.0  ! TER 2549
.C3H5Y+R2OH=>C3H5OHY    1.0E+13  0.0  0.0  ! TER 2550
.C3H5Y+R3O2H=>C3H5OOHY    5.0E+12  0.0  0.0  ! TER 2551
.C3H5Y+R4CH3=>C4H8Y    1.0E+13  0.0  0.0  ! TER 2552
.C3H5Y+R5CHO=>C3H5CHOY    1.0E+13  0.0  0.0  ! TER 2553
.C3H5Y+R6CH2OH=>C4H7OHY    1.0E+13  0.0  0.0  ! TER 2554
.C3H5Y+R11C2H5=>C5H10Y    1.0E+13  0.0  0.0  ! TER 2555
.C4H7Y+R1H=>C4H8Y    1.0E+13  0.0  0.0  ! TER 2556
.C4H7Y+R2OH=>C4H7OHY    1.0E+13  0.0  0.0  ! TER 2557
.C4H7Y+R3O2H=>C4H7OOHY    5.0E+12  0.0  0.0  ! TER 2558
.C4H7Y+R4CH3=>C5H10Y    1.0E+13  0.0  0.0  ! TER 2559
.C4H7Y+R5CHO=>C4H7CHOY    1.0E+13  0.0  0.0  ! TER 2560
.C4H7Y+R6CH2OH=>C5H9OHZ    1.0E+13  0.0  0.0  ! TER 2561
.C4H7Y+R11C2H5=>C6H12Z    1.0E+13  0.0  0.0  ! TER 2562
.C5H9Y+R1H=>C5H10Y    1.0E+13  0.0  0.0  ! TER 2563
.C5H9Y+R2OH=>C5H9OHZ    1.0E+13  0.0  0.0  ! TER 2564
.C5H9Y+R3O2H=>C5H9OOHZ    5.0E+12  0.0  0.0  ! TER 2565
.C5H9Y+R4CH3=>C6H12Z    1.0E+13  0.0  0.0  ! TER 2566
.C5H9Y+R5CHO=>C5H9CHOY    1.0E+13  0.0  0.0  ! TER 2567
.C5H9Y+R6CH2OH=>C6H11OHY    1.0E+13  0.0  0.0  ! TER 2568
.C5H9Y+R11C2H5=>C7H14Y    1.0E+13  0.0  0.0  ! TER 2569
.C7H13Y+R1H=>C7H14Y    1.0E+13  0.0  0.0  ! TER 2570
.C7H13Y+R2OH=>C7H13OHY    1.0E+13  0.0  0.0  ! TER 2571
.C7H13Y+R3O2H=>C7H13OOHY    5.0E+12  0.0  0.0  ! TER 2572
.C7H13Y+R4CH3=>C8H16Y    1.0E+13  0.0  0.0  ! TER 2573
.C7H13Y+R5CHO=>C7H13CHOY    1.0E+13  0.0  0.0  ! TER 2574
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.C7H13Y+R6CH2OH=>C8H15OHY    1.0E+13  0.0  0.0  ! TER 2575
.C7H13Y+R11C2H5=>C9H18Y    1.0E+13  0.0  0.0  ! TER 2576
.C8H15Y+R1H=>C8H16Y    1.0E+13  0.0  0.0  ! TER 2577
.C8H15Y+R2OH=>C8H15OHY    1.0E+13  0.0  0.0  ! TER 2578
.C8H15Y+R3O2H=>C8H15OOHY    5.0E+12  0.0  0.0  ! TER 2579
.C8H15Y+R4CH3=>C9H18Y    1.0E+13  0.0  0.0  ! TER 2580
.C8H15Y+R5CHO=>C8H15CHOY    1.0E+13  0.0  0.0  ! TER 2581
.C8H15Y+R6CH2OH=>C9H17OHY    1.0E+13  0.0  0.0  ! TER 2582
.C8H15Y+R11C2H5=>C10H20Y    1.0E+13  0.0  0.0  ! TER 2583
.C3H5Y+.C3H5Y=>C6H10Y2    1.0E+13  0.0  0.0  ! TER 2584
.C3H5Y+.C4H7Y=>C7H12Y2    1.0E+13  0.0  0.0  ! TER 2585
.C3H5Y+.C5H9Y=>C8H14Y2    1.0E+13  0.0  0.0  ! TER 2586
.C3H5Y+.C7H13Y=>C10H18Y2    1.0E+13  0.0  0.0  ! TER 2587
.C3H5Y+.C8H15Y=>C11H20Y2    1.0E+13  0.0  0.0  ! TER 2588
.C4H7Y+.C4H7Y=>C8H14Y2    1.0E+13  0.0  0.0  ! TER 2589
.C4H7Y+.C5H9Y=>C9H16Y2    1.0E+13  0.0  0.0  ! TER 2590
.C4H7Y+.C7H13Y=>C11H20Y2    1.0E+13  0.0  0.0  ! TER 2591
.C4H7Y+.C8H15Y=>C12H22Y2    1.0E+13  0.0  0.0  ! TER 2592
.C5H9Y+.C5H9Y=>C10H18Y2    1.0E+13  0.0  0.0  ! TER 2593
.C5H9Y+.C7H13Y=>C12H22Y2    1.0E+13  0.0  0.0  ! TER 2594
.C5H9Y+.C8H15Y=>C13H24Y2    1.0E+13  0.0  0.0  ! TER 2595
.C7H13Y+.C7H13Y=>C14H26Y2    1.0E+13  0.0  0.0  ! TER 2596
.C7H13Y+.C8H15Y=>C15H28Y2    1.0E+13  0.0  0.0  ! TER 2597
.C8H15Y+.C8H15Y=>C16H30Y2    1.0E+13  0.0  0.0  ! TER 2598


! 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>!
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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>!

!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>!
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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!
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/
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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!
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>!
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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!
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>!
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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>!
!* 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)

!REACTIONS DE O2!
O2+M=B1O+B1O+M                   1.8E18     -1.    118.1E3 !(244,-244)<TSANG86>!
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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>!
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>!
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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
>!
!       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>!
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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>!
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>!
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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>!
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>!
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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>
!
!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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