

ELEMENTS  
H O C N HE AR  
END  
SPECIES  
! 202 especes  
! Biradicals from the base :  
B1O  
B2CO  
B3C  
B4CH  
B5CH2  
B6CH2

! Molecules from the base  
H2  
H2O  
O2  
H2O2  
CH4  
HCHO  
CH3OH  
CO2  
CH3OOH  
C2H2T  
C2H4Z  
C2H6  
CH2COZ  
CH3CHO  
C2H5OH  
C2H5OOH  
CH3COOOH  
C3H6Y  
C3H8  
nC4H8Y  
C4H10  
C2H5CHO  
C3H7OH  
C2H6CO  
C3H8CO  
C4H6Z2-13  
C2H3CHOZ  
C2H4OE#3

! Radicals from the base  
R1H ! .h  
R2OH ! .oh  
R3OOH ! .o/oh  
R4CH3 ! .ch3  
R5CHO ! .ch//o  
R6CH2OH ! .ch2/oh  
R7CH3O ! .o/ch3  
R8CH3OO ! .o/o/ch3  
R9C2HT ! .c///ch  
R10C2H3V ! .ch//ch2  
R11C2H5 ! .ch2/ch3  
R12CHCOV ! .ch//c//o  
R13CH2CHO ! .ch2/ch//o  
R14CH3CO ! .c(//o)/ch3

R15C2H5O ! .o/ch2/ch3  
R16C2H4OOH ! .ch2/ch2/o/oh  
R17C2H5OO ! .o/o/ch2/ch3  
R18CH3COOO ! .o/o/c(/o)/ch3  
R19C3H7 ! .ch2/ch2/ch3  
R20C4H9 ! .ch2/ch2/ch2/ch3  
R21CH3OCO ! .c(/o)/o/ch3  
R22CO2H ! .c(/o)/oh  
R23C2H3O2B ! .ch2/c(/o)/oh  
R24C2H4OH ! .ch2/ch2/oh  
R25C2H4OH ! .ch(/oh)/ch3

! Primary molecules :

! Reactants:

C5H12-1  
C6H12OA-1  
C6H12O2B-1  
C4H8OA  
C5H10OA  
C5H10OK  
C6H10O2A  
C6H10O2KA  
C6H10O3AB  
C6H10O3KB  
C3H6O3KP  
C4H8O3KP  
C5H10O3KP  
C6H10O4KAP  
C6H10O5KPB  
C4H6O4KAP  
C3H4O4KAP  
C4H6O5KPB  
C3H4O5KPB  
M31C5H10Y  
M32C5H10Z  
M38C6H10OAZ  
M35C6H10OAZ  
M34C6H10OAZ  
M33C6H10OAZ  
C5H8OAZ  
C4H6OAZ  
M39C6H10OKZ  
M45C6H10O2ZB  
M42C6H10O2ZB  
M41C6H10O2ZB  
M40C6H10O2ZB  
C5H8O2ZB  
C4H6O2ZB  
C3H4O2ZB  
C5H12O2P  
C6H12O3AP  
C6H12O4PB  
C3H6O2PZ  
C4H8O2PZ  
C5H10O2PZ  
C5H8O3APZ  
C4H6O3APZ  
C3H4O3APZ  
C6H10O3KPZ

C5H8O4PZB  
C4H6O4PZB  
C3H4O4PZB  
C4H6O2A2  
C3H4O2A2  
C4H6O3KPZ  
C3H4O3KPZ  
C4H6O3AB  
C3H4O3AB  
C3H4OKZ  
C4H6OKZ  
C3H8OL  
C3H8O2P  
C4H10  
C4H10OL  
M102C5H12  
C6H14  
C4H10O2P  
C4H8O3AP  
C3H6O3AP  
C4H8O4PB  
C3H6O4PB

! Secondary molecules :

C4H6Z2  
C4H8Z  
C4H8Y  
C6H12Z  
C7H14Z  
C8H16Z  
C6H12OA  
C7H14OA  
C5H8Z2  
C3H4Z2  
C3H6OLY  
C3H6O2PY  
C4H6OAY  
C4H8OLY  
C6H10Y2  
C7H12Y2  
C8H14Y2  
C4H8O2PY  
C5H8OAY  
C5H10OLY  
C9H16Y2  
C5H10O2PY  
C6H10OAY  
C6H12OLY  
C10H18Y2  
C3H6Z

! Cyclic primary molecules :

C3H6OE#3  
C3H6OE#4  
C4H8OE#3  
C4H8OE#4  
C4H8OE#5  
M9C5H10OE#3

M7C5H10OE#3

M12C5H10OE#4  
M8C5H10OE#4

!M10C5H10OE#5

M11C5H10OE#6

M22C6H10O2E#3A  
M20C6H10O2E#3A  
M17C6H10O2E#3A  
M13C6H10O2E#3A

M21C6H10O2E#4A  
M18C6H10O2E#4A  
M14C6H10O2E#4A

M19C6H10O2E#5A  
M15C6H10O2E#5A

M16C6H10O2E#6A

M32C6H10O3E#3LK  
M30C6H10O3E#3LK  
M27C6H10O3E#3LK  
M23C6H10O3E#3LK

M31C6H10O3E#4LK  
M28C6H10O3E#4LK  
M24C6H10O3E#4LK

M29C6H10O3E#5LK  
M25C6H10O3E#5LK

M26C6H10O3E#6LK

C4H6O2E#3A  
C4H6O2E#4A  
C3H4O2E#3A  
C4H6O3E#3LK  
C4H6O3E#4LK  
C3H4O3E#3LK

! Cyclic secondary molecules :

C6H12OE#3  
C7H14OE#3  
C8H16OE#3  
C5H8O4E#4KP  
C5H8O4E#5KP  
C5H8O4E#6KP

! Benzenic primary molecules :

! Benzenic cyclo ether primary molecules :

! Free radicals :

R26C5H11 ! .ch(/ch2/ch3)2  
R27C5H11 ! .ch2/ch2/ch2/ch2/ch3

R28C5H11 ! .ch(/ch3)/ch2/ch2/ch3  
R29C6H11OK ! .c(/o)/ch2/ch2/ch2/ch2/ch3  
R30C6H11OA ! .ch2/ch2/ch2/ch2/ch2/ch//o  
R31C6H11OA ! .ch(/ch3)/ch2/ch2/ch2/ch//o  
R32C6H11OA ! .ch(/ch2/ch3)/ch2/ch2/ch//o  
R33C6H11OA ! .ch(/ch2/ch//o)/ch2/ch2/ch3  
R34C6H11OA ! .ch(/ch//o)/ch2/ch2/ch2/ch3  
R35C6H11O2K ! .o/c(/o)/ch2/ch2/ch2/ch2/ch3  
R36C6H11O2B ! .ch2/ch2/ch2/ch2/ch2/c(/o)/oh  
R37C6H11O2B ! .ch(/ch3)/ch2/ch2/ch2/c(/o)/oh  
R38C6H11O2B ! .ch(/ch2/ch3)/ch2/ch2/c(/o)/oh  
R39C6H11O2B ! .ch(/ch2/c(/o)/oh)/ch2/ch2/ch3  
R40C6H11O2B ! .ch(/c(/o)/oh)/ch2/ch2/ch2/ch3  
R41C3H7O2U ! .o/o/ch2/ch2/ch3  
R42C4H9O2U ! .o/o/ch2/ch2/ch2/ch3  
R43C5H11O2U ! .o/o/ch(/ch2/ch3)2  
R44C5H11O2U ! .o/o/ch2/ch2/ch2/ch2/ch3  
R45C5H11O2U ! .o/o/ch(/ch3)/ch2/ch2/ch3  
R46C6H11O3AU ! .o/o/ch2/ch2/ch2/ch2/ch2/ch//o  
R47C4H7OA ! .ch2/ch2/ch2/ch//o  
R48C6H11O3AU ! .o/o/ch(/ch3)/ch2/ch2/ch2/ch//o  
R49C3H5OA ! .ch2/ch2/ch//o  
R50C6H11O3AU ! .o/o/ch(/ch2/ch3)/ch2/ch2/ch//o  
R51C6H11O3AU ! .o/o/ch(/ch2/ch//o)/ch2/ch2/ch3  
R52C6H11O3AU ! .o/o/ch(/ch//o)/ch2/ch2/ch2/ch3  
R53C6H11O4UB ! .o/o/ch2/ch2/ch2/ch2/ch2/c(/o)/oh  
R54C4H7O2B ! .ch2/ch2/ch2/c(/o)/oh  
R55C6H11O4UB ! .o/o/ch(/ch3)/ch2/ch2/ch2/c(/o)/oh  
R56C3H5O2B ! .ch2/ch2/c(/o)/oh  
R57C6H11O4UB ! .o/o/ch(/ch2/ch3)/ch2/ch2/c(/o)/oh  
R58C6H11O4UB ! .o/o/ch(/ch2/c(/o)/oh)/ch2/ch2/ch3  
R59C6H11O4UB ! .o/o/ch(/c(/o)/oh)/ch2/ch2/ch2/ch3  
R60C3H7O2P ! .ch(/ch3)/ch2/o/oh  
R61C3H7O2P ! .ch2/ch2/ch2/o/oh  
R62C4H9O2P ! .ch(/ch2/o/oh)/ch2/ch3  
R63C4H9O2P ! .ch(/ch3)/ch2/ch2/o/oh  
R64C4H9O2P ! .ch2/ch2/ch2/ch2/o/oh  
R65C5H11O2P ! .ch(/ch3)/ch(/o/oh)/ch2/ch3  
R66C5H11O2P ! .ch2/ch2/ch(/o/oh)/ch2/ch3  
R67C5H11O2P ! .ch(/ch2/o/oh)/ch2/ch2/ch3  
R68C5H11O2P ! .ch(/ch2/ch3)/ch2/ch2/o/oh  
R69C5H11O2P ! .ch(/ch3)/ch2/ch2/ch2/o/oh  
R70C5H11O2P ! .ch2/ch2/ch2/ch2/ch2/o/oh  
R71C5H11O2P ! .ch2/ch(/o/oh)/ch2/ch2/ch3  
R72C5H11O2P ! .ch(/ch2/ch3)/ch(/o/oh)/ch3  
R73C5H11O2P ! .ch(/ch3)/ch2/ch(/o/oh)/ch3  
R74C5H11O2P ! .ch2/ch2/ch2/ch(/o/oh)/ch3  
R75C6H11O3AP ! .ch(/ch2/o/oh)/ch2/ch2/ch2/ch//o  
R76C6H11O3AP ! .ch(/ch2/ch2/o/oh)/ch2/ch2/ch//o  
R77C6H11O3AP ! .ch(/ch2/ch//o)/ch2/ch2/ch2/o/oh  
R78C6H11O3AP ! .ch(/ch//o)/ch2/ch2/ch2/ch2/o/oh  
R79C4H7O3AU ! .o/o/ch2/ch2/ch2/ch//o  
R80C4H7OK ! .c(/o)/ch2/ch2/ch3  
R81C6H11O3AP ! .ch2/ch(/o/oh)/ch2/ch2/ch2/ch//o  
R82C6H11O3AP ! .ch(/ch(/o/oh)/ch3)/ch2/ch2/ch//o  
R83C6H11O3AP ! .ch(/ch2/ch//o)/ch2/ch(/o/oh)/ch3  
R84C6H11O3AP ! .ch(/ch//o)/ch2/ch2/ch(/o/oh)/ch3  
R85C6H11O3KP ! .c(/o)/ch2/ch2/ch2/ch(/o/oh)/ch3

R86C3H5O3AU ! .o/o/ch2/ch2/ch//o  
R87C6H11O3AP ! .ch(/ch3)/ch(/o/oh)/ch2/ch2/ch//o  
R88C6H11O3AP ! .ch2/ch2/ch(/o/oh)/ch2/ch2/ch//o  
R89C6H11O3AP ! .ch(/ch2/ch//o)/ch(/o/oh)/ch2/ch3  
R90C6H11O3AP ! .ch(/ch//o)/ch2/ch(/o/oh)/ch2/ch3  
R91C6H11O3KP ! .c(/o)/ch2/ch2/ch(/o/oh)/ch2/ch3  
R92C6H11O3AP ! .ch(/ch//o)/ch(/o/oh)/ch2/ch2/ch3  
R93C6H11O3KP ! .c(/o)/ch2/ch(/o/oh)/ch2/ch2/ch3  
R94C6H11O3AP ! .ch(/ch2/ch3)/ch(/o/oh)/ch2/ch//o  
R95C6H11O3AP ! .ch(/ch3)/ch2/ch(/o/oh)/ch2/ch//o  
R96C6H11O3AP ! .ch2/ch2/ch2/ch(/o/oh)/ch2/ch//o  
R97C6H11O3KP ! .c(/o)/ch(/o/oh)/ch2/ch2/ch2/ch3  
R98C6H11O3AP ! .ch(/ch(/o/oh)/ch//o)/ch2/ch2/ch3  
R99C6H11O3AP ! .ch(/ch2/ch3)/ch2/ch(/o/oh)/ch//o  
R100C6H11O3AP ! .ch(/ch3)/ch2/ch2/ch(/o/oh)/ch//o  
R101C6H11O3AP ! .ch2/ch2/ch2/ch2/ch(/o/oh)/ch//o  
R102C6H11O4PB ! .ch(/ch2/o/oh)/ch2/ch2/ch2/c(/o)/oh  
R103C6H11O4PB ! .ch(/ch2/ch2/o/oh)/ch2/ch2/c(/o)/oh  
R104C6H11O4PB ! .ch(/ch2/c(/o)/oh)/ch2/ch2/ch2/o/oh  
R105C6H11O4PB ! .ch(/c(/o)/oh)/ch2/ch2/ch2/ch2/o/oh  
R106C4H7O4UB ! .o/o/ch2/ch2/ch2/c(/o)/oh  
R107C6H11O4PB ! .ch2/ch(/o/oh)/ch2/ch2/ch2/c(/o)/oh  
R108C6H11O4PB ! .ch(/ch(/o/oh)/ch3)/ch2/ch2/c(/o)/oh  
R109C6H11O4PB ! .ch(/ch2/c(/o)/oh)/ch2/ch(/o/oh)/ch3  
R110C6H11O4PB ! .ch(/c(/o)/oh)/ch2/ch2/ch(/o/oh)/ch3  
R111C3H5O4UB ! .o/o/ch2/ch2/c(/o)/oh  
R112C6H11O4PB ! .ch(/ch3)/ch(/o/oh)/ch2/ch2/c(/o)/oh  
R113C6H11O4PB ! .ch2/ch2/ch(/o/oh)/ch2/ch2/c(/o)/oh  
R114C6H11O4PB ! .ch(/ch2/c(/o)/oh)/ch(/o/oh)/ch2/ch3  
R115C6H11O4PB ! .ch(/c(/o)/oh)/ch2/ch(/o/oh)/ch2/ch3  
R116C6H11O4PB ! .ch(/c(/o)/oh)/ch(/o/oh)/ch2/ch2/ch3  
R117C6H11O4PB ! .ch(/ch2/ch3)/ch(/o/oh)/ch2/c(/o)/oh  
R118C6H11O4PB ! .ch(/ch3)/ch2/ch(/o/oh)/ch2/c(/o)/oh  
R119C6H11O4PB ! .ch2/ch2/ch2/ch(/o/oh)/ch2/c(/o)/oh  
R120C6H11O4PB ! .ch(/ch(/o/oh)/c(/o)/oh)/ch2/ch2/ch3  
R121C6H11O4PB ! .ch(/ch2/ch3)/ch2/ch(/o/oh)/c(/o)/oh  
R122C6H11O4PB ! .ch(/ch3)/ch2/ch2/ch(/o/oh)/c(/o)/oh  
R123C6H11O4PB ! .ch2/ch2/ch2/ch2/ch(/o/oh)/c(/o)/oh  
R124C3H7O4UP ! .o/o/ch(/ch3)/ch2/o/oh  
R125C3H7O4UP ! .o/o/ch2/ch2/ch2/o/oh  
R126C4H9O4UP ! .o/o/ch(/ch2/o/oh)/ch2/ch3  
R127C4H9O4UP ! .o/o/ch(/ch3)/ch2/ch2/o/oh  
R128C4H9O4UP ! .o/o/ch2/ch2/ch2/ch2/o/oh  
R129C5H11O4UP ! .o/o/ch(/ch3)/ch(/o/oh)/ch2/ch3  
R130C5H11O4UP ! .o/o/ch2/ch2/ch(/o/oh)/ch2/ch3  
R131C3H7O2P ! .ch(/o/oh)/ch2/ch3  
R132C5H11O4UP ! .o/o/ch(/ch2/o/oh)/ch2/ch2/ch3  
R133C5H11O4UP ! .o/o/ch(/ch2/ch3)/ch2/ch2/o/oh  
R134C5H11O4UP ! .o/o/ch(/ch3)/ch2/ch2/ch2/o/oh  
R135C5H11O4UP ! .o/o/ch2/ch2/ch2/ch2/o/oh  
R136C5H11O4UP ! .o/o/ch2/ch(/o/oh)/ch2/ch2/ch3  
R137C5H11O4UP ! .o/o/ch(/ch2/ch3)/ch(/o/oh)/ch3  
R138C5H11O4UP ! .o/o/ch(/ch3)/ch2/ch(/o/oh)/ch3  
R139C5H11O4UP ! .o/o/ch2/ch2/ch2/ch(/o/oh)/ch3  
R140C3H7O2P ! .ch2/ch(/o/oh)/ch3  
R141C6H11O5AUP ! .o/o/ch(/ch2/o/oh)/ch2/ch2/ch2/ch//o  
R142C6H11O3KP ! .c(/o)/ch2/ch2/ch2/ch2/o/oh  
R143C6H11O5AUP ! .o/o/ch(/ch2/ch2/o/oh)/ch2/ch2/ch//o

R144C6H11O5AUP ! .o/o/ch (/ch2/ch//o) /ch2/ch2/ch2/o/oh  
R145C6H11O5AUP ! .o/o/ch (/ch//o) /ch2/ch2/ch2/ch2/o/oh  
R146C4H7O3AP ! .ch (/ch2/o/oh) /ch2/ch//o  
R147C4H7O3AP ! .ch (/ch//o) /ch2/ch2/o/oh  
R148C4H7O3KP ! .c (/o) /ch2/ch2/ch2/o/oh  
R149C6H11O5AUP ! .o/o/ch2/ch (/o/oh) /ch2/ch2/ch2/ch//o  
R150C6H11O5AUP ! .o/o/ch (/ch (/o/oh) /ch3) /ch2/ch2/ch//o  
R151C6H11O5AUP ! .o/o/ch (/ch2/ch//o) /ch2/ch (/o/oh) /ch3  
R152C6H11O5AUP ! .o/o/ch (/ch//o) /ch2/ch2/ch (/o/oh) /ch3  
R153C3H5O3AP ! .ch (/ch//o) /ch2/o/oh  
R154C3H5O3KP ! .c (/o) /ch2/ch2/o/oh  
R155C6H11O5AUP ! .o/o/ch (/ch3) /ch (/o/oh) /ch2/ch2/ch//o  
R156C6H11O5AUP ! .o/o/ch2/ch2/ch (/o/oh) /ch2/ch2/ch//o  
R157C4H7O3AP ! .ch (/o/oh) /ch2/ch2/ch//o  
R158C6H11O5AUP ! .o/o/ch (/ch2/ch//o) /ch (/o/oh) /ch2/ch3  
R159C6H11O5AUP ! .o/o/ch (/ch//o) /ch2/ch (/o/oh) /ch2/ch3  
R160C6H11O5AUP ! .o/o/ch (/ch//o) /ch (/o/oh) /ch2/ch2/ch3  
R161C6H11O5AUP ! .o/o/ch (/ch2/ch3) /ch (/o/oh) /ch2/ch//o  
R162C6H11O5AUP ! .o/o/ch (/ch3) /ch2/ch (/o/oh) /ch2/ch//o  
R163C3H5O3AP ! .ch (/o/oh) /ch2/ch//o  
R164C6H11O5AUP ! .o/o/ch2/ch2/ch2/ch (/o/oh) /ch2/ch//o  
R165C4H7O3AP ! .ch2/ch (/o/oh) /ch2/ch//o  
R166C5H11O2P ! .ch (/o/oh) /ch2/ch2/ch2/ch3  
R167C6H11O5AUP ! .o/o/ch (/ch (/o/oh) /ch//o) /ch2/ch2/ch3  
R168C6H11O5AUP ! .o/o/ch (/ch2/ch3) /ch2/ch (/o/oh) /ch//o  
R169C6H11O5AUP ! .o/o/ch (/ch3) /ch2/ch2/ch (/o/oh) /ch//o  
R170C3H5O3AP ! .ch2/ch (/o/oh) /ch//o  
R171C6H11O5AUP ! .o/o/ch2/ch2/ch2/ch2/ch (/o/oh) /ch//o  
R172C4H7O3AP ! .ch2/ch2/ch (/o/oh) /ch//o  
R173C6H11O6UPB ! .o/o/ch (/ch2/o/oh) /ch2/ch2/ch2/c (/o) /oh  
R174C6H11O6UPB ! .o/o/ch (/ch2/ch2/o/oh) /ch2/ch2/c (/o) /oh  
R175C6H11O6UPB ! .o/o/ch (/ch2/c (/o) /oh) /ch2/ch2/ch2/o/oh  
R176C6H11O6UPB ! .o/o/ch (/c (/o) /oh) /ch2/ch2/ch2/ch2/o/oh  
R177C4H7O4PB ! .ch (/ch2/o/oh) /ch2/c (/o) /oh  
R178C4H7O4PB ! .ch (/c (/o) /oh) /ch2/ch2/o/oh  
R179C6H11O6UPB ! .o/o/ch2/ch (/o/oh) /ch2/ch2/ch2/c (/o) /oh  
R180C6H11O6UPB ! .o/o/ch (/ch (/o/oh) /ch3) /ch2/ch2/c (/o) /oh  
R181C6H11O6UPB ! .o/o/ch (/ch2/c (/o) /oh) /ch2/ch (/o/oh) /ch3  
R182C6H11O6UPB ! .o/o/ch (/c (/o) /oh) /ch2/ch2/ch (/o/oh) /ch3  
R183C3H5O4PB ! .ch (/c (/o) /oh) /ch2/o/oh  
R184C6H11O6UPB ! .o/o/ch (/ch3) /ch (/o/oh) /ch2/ch2/c (/o) /oh  
R185C6H11O6UPB ! .o/o/ch2/ch2/ch (/o/oh) /ch2/ch2/c (/o) /oh  
R186C4H7O4PB ! .ch (/o/oh) /ch2/ch2/c (/o) /oh  
R187C6H11O6UPB ! .o/o/ch (/ch2/c (/o) /oh) /ch (/o/oh) /ch2/ch3  
R188C6H11O6UPB ! .o/o/ch (/c (/o) /oh) /ch2/ch (/o/oh) /ch2/ch3  
R189C6H11O6UPB ! .o/o/ch (/c (/o) /oh) /ch (/o/oh) /ch2/ch2/ch3  
R190C6H11O6UPB ! .o/o/ch (/ch2/ch3) /ch (/o/oh) /ch2/c (/o) /oh  
R191C6H11O6UPB ! .o/o/ch (/ch3) /ch2/ch (/o/oh) /ch2/c (/o) /oh  
R192C3H5O4PB ! .ch (/o/oh) /ch2/c (/o) /oh  
R193C6H11O6UPB ! .o/o/ch2/ch2/ch2/ch (/o/oh) /ch2/c (/o) /oh  
R194C4H7O4PB ! .ch2/ch (/o/oh) /ch2/c (/o) /oh  
R195C6H11O6UPB ! .o/o/ch (/ch (/o/oh) /c (/o) /oh) /ch2/ch2/ch3  
R196C6H11O6UPB ! .o/o/ch (/ch2/ch3) /ch2/ch (/o/oh) /c (/o) /oh  
R197C6H11O6UPB ! .o/o/ch (/ch3) /ch2/ch2/ch (/o/oh) /c (/o) /oh  
R198C3H5O4PB ! .ch2/ch (/o/oh) /c (/o) /oh  
R199C6H11O6UPB ! .o/o/ch2/ch2/ch2/ch2/ch (/o/oh) /c (/o) /oh  
R200C4H7O4PB ! .ch2/ch2/ch (/o/oh) /c (/o) /oh  
R201C3H7O4UP ! .o/o/ch (/o/oh) /ch2/ch3

R202C3H7O4UP ! .o/o/ch2/ch(/o/oh)/ch3  
R203C3H7O2U ! .o/o/ch(/ch3)2  
R204C4H7O5AUP ! .o/o/ch(/ch2/o/oh)/ch2/ch//o  
R205C4H7O5AUP ! .o/o/ch(/ch//o)/ch2/ch2/o/oh  
R206C3H5O5AUP ! .o/o/ch(/ch//o)/ch2/o/oh  
R207C4H7O5AUP ! .o/o/ch(/o/oh)/ch2/ch2/ch//o  
R208C3H5O5AUP ! .o/o/ch(/o/oh)/ch2/ch//o  
R209C4H7O5AUP ! .o/o/ch2/ch(/o/oh)/ch2/ch//o  
R210C4H7O3AU ! .o/o/ch(/ch3)/ch2/ch//o  
R211C4H7O3KP ! .c(/o)/ch2/ch(/o/oh)/ch3  
R212C5H11O4UP ! .o/o/ch(/o/oh)/ch2/ch2/ch2/ch3  
R213C3H5O5AUP ! .o/o/ch2/ch(/o/oh)/ch//o  
R214C3H5O3AU ! .o/o/ch(/ch3)/ch//o  
R215C4H7O5AUP ! .o/o/ch2/ch2/ch(/o/oh)/ch//o  
R216C4H7O3AU ! .o/o/ch(/ch//o)/ch2/ch3  
R217C4H7O3KP ! .c(/o)/ch(/o/oh)/ch2/ch3  
R218C4H7O6UPB ! .o/o/ch(/ch2/o/oh)/ch2/c(/o)/oh  
R219C4H7O6UPB ! .o/o/ch(/c(/o)/oh)/ch2/ch2/o/oh  
R220C3H5O6UPB ! .o/o/ch(/c(/o)/oh)/ch2/o/oh  
R221C4H7O6UPB ! .o/o/ch(/o/oh)/ch2/ch2/c(/o)/oh  
R222C3H5O6UPB ! .o/o/ch(/o/oh)/ch2/c(/o)/oh  
R223C4H7O6UPB ! .o/o/ch2/ch(/o/oh)/ch2/c(/o)/oh  
R224C4H7O4UB ! .o/o/ch(/ch3)/ch2/c(/o)/oh  
R225C3H5O6UPB ! .o/o/ch2/ch(/o/oh)/c(/o)/oh  
R226C3H5O4UB ! .o/o/ch(/ch3)/c(/o)/oh  
R227C4H7O6UPB ! .o/o/ch2/ch2/ch(/o/oh)/c(/o)/oh  
R228C4H7O4UB ! .o/o/ch(/c(/o)/oh)/ch2/ch3  
R229C3H7 ! .ch(/ch3)2  
R230C4H7O3AP ! .ch(/ch//o)/ch(/o/oh)/ch3  
R231C4H7OA ! .ch(/ch3)/ch2/ch//o  
R232C3H5O3KP ! .c(/o)/ch(/o/oh)/ch3  
R233C3H5OA ! .ch(/ch3)/ch//o  
R234C4H7O3AP ! .ch(/ch3)/ch(/o/oh)/ch//o  
R235C4H7OA ! .ch(/ch//o)/ch2/ch3  
R236C4H7O4PB ! .ch(/c(/o)/oh)/ch(/o/oh)/ch3  
R237C4H7O2B ! .ch(/ch3)/ch2/c(/o)/oh  
R238C3H5O2B ! .ch(/ch3)/c(/o)/oh  
R239C4H7O4PB ! .ch(/ch3)/ch(/o/oh)/c(/o)/oh  
R240C4H7O2B ! .ch(/c(/o)/oh)/ch2/ch3  
R241C4H7O5AUP ! .o/o/ch(/ch//o)/ch(/o/oh)/ch3  
R242C4H7O5AUP ! .o/o/ch(/ch3)/ch(/o/oh)/ch//o  
R243C4H7O6UPB ! .o/o/ch(/c(/o)/oh)/ch(/o/oh)/ch3  
R244C4H7O6UPB ! .o/o/ch(/ch3)/ch(/o/oh)/c(/o)/oh  
R245C5H9OA ! .ch2/ch2/ch2/ch2/ch//o  
R246C5H9O2B ! .ch2/ch2/ch2/ch2/c(/o)/oh

!Cyclic free radicals:

!Benzenic free radicals:

! lumped Free radicals :

RC3H5Y  
RC4H7Y  
RC3H5O  
RC5H9O  
RC5H9Y  
RC6H9OZ  
RC5H7OZ  
RC4H5OZ  
RC3H5O3



RC5H9O3  
RC6H9O3Z  
RC5H7O3Z  
RC4H5O3Z  
RC7H13O  
RC6H13  
RC7H13O3  
! lumped Cyclic free radicals :

C5H9OE#4  
C5H9OE#5  
C5H9OE#6  
C5H9O3E#4U  
C5H9O3E#5U  
C5H9O3E#6U  
C5H9O3E#4P  
C5H9O3E#5P  
C5H9O3E#6P  
C5H9O5E#4UP  
C5H9O5E#5UP  
C5H9O5E#6UP

N2  
HE  
AR

!Added species

R290C6H11O3AU !ch3/ch2/ch2/ch2/ch2/c(/o/o(.))//o  
R291C6H11O3AP !ch3/ch2/ch2/ch(/o/o(.))/ch2/c(/o/oh)//o  
R292C6H11O3AP !ch3/ch2/ch(/o/o(.))/ch2/ch2/c(/o/oh)//o  
R293C6H11O3AP !ch3/ch(/o/o(.))/ch2/ch2/ch2/c(/o/oh)//o  
R300C6H11O5APU !ch3/ch2/ch2/ch(/o/o(.))/ch2/c(/o/oh)//o  
R301C6H11O5APU !ch3/ch2/ch(/o/o(.))/ch2/ch2/c(/o/oh)//o  
R302C6H11O5APU !ch3/ch(/o/o(.))/ch2/ch2/ch2/c(/o/oh)//o  
R305C6H11O5APP !ch3/ch(/o/o(.))/ch2/ch(/o/oh)/ch2/c(/o/oh)//o  
R306C6H11O5APP  
R307C6H11O5APP  
R310C6H11O7APPU !ch3/ch(/o/o(.))/ch2/ch(/o/oh)/ch2/c(/o/oh)//o  
R311C6H11O7APPU  
R312C6H11O7APPU  
C6H8OK(OOH)20 !ch3/ch(/o/oh)/ch2/c(/o/oh)/ch2/c(/o/oh)//o  
C6H11OKOOH !ch3/ch2/ch2/ch2/ch2/c(/o/oh)//o  
gcaprolac ! ch2(#1)/ch(/ch2/ch3)/o/c(/o/oh)/ch2/1  
dcaprolac ! ch2(#1)/ch(/ch3)/o/c(/o/oh)/ch2/ch2/1  
  
C6H12OOHP !ch3/ch2/ch2/ch2/ch2/ch(/o/oh)/o(.)  
HCOOOH !ch(/o/oh)/o/oh  
C6H11OKOH !ch3/ch2/ch2/ch2/ch2/ch(/oh)/o(.)  
HCOOH  
M10C5H10OE#5  
C6H11OKO ! ch3/ch2/ch2/ch2/ch2/c(/o/oh)/o(.)

!Species specific to 1-hexanol

C6H14OL-1  
C6H12OLZ

R32C6H13OL  
R33C6H13O  
R34C6H13OL

R35C6H13OL  
R36C6H13OL  
R37C6H13OL  
R38C6H13OL

R51C6H13O3LU

R53C4H9OL  
R55C3H7OL

R302C6H13  
R303C5H11OL

END

THERMO ALL ! Nasa coefficients validated

300.000 1000.000 5000.000  
N2 Ranzi ON 2C OH OO OG 0300.00 5000.00 1000.00  
1  
0.29266379E+01 0.14879770E-02-0.56847603E-06 0.10097040E-09-0.67533509E-  
14 2  
-0.92279538E+03 0.59805402E+01 0.32986770E+01 0.14082399E-02-0.39632218E-  
05 3  
0.56415148E-08-0.24448540E-11-0.10209000E+04 0.39503720E+01  
4  
HE Ranzi OHE 2C OH OO OG 0300.00 5000.00 1000.00  
1  
0.31250001E+01-0.14062505E-02 0.93750049E-06-0.15625008E-09  
0.00000000E+00 2  
-0.94068758E+03-0.24124152E+01 0.25000000E+01 0.00000000E+00  
0.00000000E+00 3  
0.00000000E+00 0.00000000E+00-0.74537510E+03 0.91534890E+00  
4  
AR 120186AR 1 G 0300.00 5000.00 1000.00  
1  
0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00  
0.00000000E+00 2  
-0.74537500E+03 0.43660010E+01 0.25000000E+01 0.00000000E+00  
0.00000000E+00 3  
0.00000000E+00 0.00000000E+00-0.74537500E+03 0.43660010E+01  
4  
B10 O 1 G 0300.00 5000.00 1000.00  
1  
0.25420608E+01-0.27550620E-04-0.31028030E-08 0.45510670E-11-0.43680520E-  
15 2  
0.29230798E+05 0.49203024E+01 0.29464290E+01-0.16381660E-02 0.24210320E-  
05 3  
-0.16028430E-08 0.38906960E-12 0.29147640E+05 0.29639950E+01  
4  
B2CO C 1O 1 G 0300.00 5000.00 1000.00  
1  
0.30250777E+01 0.14426890E-02-0.56308280E-06 0.10185810E-09-0.69109520E-  
14 2  
-0.14268350E+05 0.61082221E+01 0.32624520E+01 0.15119410E-02-0.38817550E-  
05 3  
0.55819440E-08-0.24749510E-11-0.14310540E+05 0.48488970E+01  
4

B3C C 1 G 0300.00 5000.00 1000.00  
 1  
 0.26020867E+01-0.17870810E-03 0.90870410E-07-0.11499330E-10 0.33108440E-15 2  
 0.85421542E+05 0.41951820E+01 0.24985850E+01 0.80857770E-04-0.26976970E-06 3  
 0.30407290E-09-0.11066520E-12 0.85458780E+05 0.47534590E+01  
 4  
 B4CH C 1H 1 G 0300.00 5000.00 1000.00  
 1  
 0.21962223E+01 0.23403810E-02-0.70582010E-06 0.90075820E-10-0.38550400E-14 2  
 0.70867231E+05 0.91783754E+01 0.32002020E+01 0.20728760E-02-0.51344310E-05 3  
 0.57338900E-08-0.19555330E-11 0.70452590E+05 0.33315880E+01  
 4  
 B5CH2 CH2t C 1H 2 G 0300.00 5000.00 1000.00  
 1  
 0.36364065E+01 0.19330570E-02-0.16870160E-06-0.10098990E-09 0.18082560E-13 2  
 0.45341345E+05 0.21565691E+01 0.37622370E+01 0.11598190E-02 0.24895850E-06 3  
 0.88008360E-09-0.73324350E-12 0.45367910E+05 0.17125780E+01  
 4  
 B6CH2 CH2s C 1H 2 G 0300.00 5000.00 1000.00  
 1  
 0.35528875E+01 0.20667880E-02-0.19141160E-06-0.11046730E-09 0.20213500E-13 2  
 0.49849761E+05 0.16865777E+01 0.39712650E+01-0.16990890E-03 0.10253690E-05 3  
 0.24925510E-08-0.19812660E-11 0.49893680E+05 0.57532070E-01  
 4  
 H2 C 0H 2O 0 G 0300.00 5000.00 1000.00  
 1  
 0.24971474E+01 0.17808300E-02-0.78001300E-06 0.14843700E-09-0.10340100E-13 2  
 -0.68234235E+03 0.12869436E+01 0.34385300E+01 0.14431400E-03-0.10819100E-06 3  
 0.21683900E-09-0.55430700E-13-0.10374900E+04-0.39268200E+01  
 4  
 H2O C 0H 2O 1 G 0300.00 5000.00 1000.00  
 1  
 0.26801061E+01 0.30962300E-02-0.93139300E-06 0.13486500E-09-0.77000700E-14 2  
 -0.29923344E+05 0.67805263E+01 0.39755900E+01-0.44183400E-03 0.24559600E-05 3  
 -0.12443100E-08 0.22670200E-12-0.30281000E+05 0.77152300E-01  
 4  
 O2 C 0H 0O 2 G 0300.00 5000.00 1000.00  
 1  
 0.31892691E+01 0.15665700E-02-0.69065700E-06 0.13208200E-09-0.92357700E-14 2  
 -0.10481021E+04 0.59950619E+01 0.30880900E+01 0.16034200E-02-0.53455000E-06 3  
 0.28079300E-10 0.29889900E-14-0.99382800E+03 0.66106900E+01  
 4  
 H2O2 C 0H 2O 2 G 0300.00 5000.00 1014.00  
 1

0.54773971E+01 0.26651844E-02-0.69380576E-06 0.91391290E-10-0.49374605E-  
 14 2  
 -0.18283678E+05-0.43962599E+01 0.25265224E+01 0.11391788E-01-0.89037285E-  
 05 3  
 0.24531213E-08 0.71861218E-13-0.17565287E+05 0.10559545E+02  
 4  
 CH4 C 1H 4O 0 G 0300.00 5000.00 1015.00  
 1  
 0.16080835E+01 0.10308000E-01-0.37122800E-05 0.61418500E-09-0.38674800E-  
 13 2  
 -0.10063071E+05 0.10071468E+02 0.23195400E+01 0.65473800E-02-0.74805100E-  
 06 3  
 0.26091200E-08-0.19553700E-11-0.99976400E+04 0.72496500E+01  
 4  
 HCHO C 1H 2O 1 G 0300.00 5000.00 1017.00  
 1  
 0.29042038E+01 0.66440700E-02-0.24528200E-05 0.41283600E-09-0.26304000E-  
 13 2  
 -0.14432160E+05 0.75065132E+01 0.24104900E+01 0.70204100E-02-0.42294700E-  
 05 3  
 0.44011600E-08-0.21264700E-11-0.14111400E+05 0.10624600E+02  
 4  
 CH3OH C 1H 4O 1 G 0300.00 5000.00 1000.00  
 1  
 0.32627246E+01 0.10543200E-01-0.35491800E-05 0.55874300E-09-0.33923600E-  
 13 2  
 -0.25878233E+05 0.67000165E+01 0.18595700E+01 0.12531200E-01-0.44710700E-  
 05 3  
 0.17329300E-08-0.87106600E-12-0.25287900E+05 0.14683500E+02  
 4  
 CO2 C 1H 0O 2 G 0300.00 5000.00 1005.00  
 1  
 0.41987613E+01 0.34902790E-02-0.14128319E-05 0.25480168E-09-0.17105678E-  
 13 2  
 -0.48815924E+05 0.56029982E+00 0.22576122E+01 0.95094619E-02-0.73198071E-  
 05 3  
 0.20577067E-08 0.10320530E-13-0.48371590E+05 0.10295759E+02  
 4  
 CH3OOH C 1H 4O 2 G 0300.00 5000.00 1000.00  
 1  
 0.63680096E+01 0.10737200E-01-0.36866600E-05 0.58882700E-09-0.36126600E-  
 13 2  
 -0.18426159E+05-0.60734207E+01 0.30921800E+01 0.18022300E-01-0.71186200E-  
 05 3  
 -0.14797800E-08 0.14551700E-11-0.17430000E+05 0.11302800E+02  
 4  
 C2H2T C 2H 2O 0 G 0300.00 5000.00 1000.00  
 1  
 0.44367752E+01 0.53760390E-02-0.19128170E-05 0.32863790E-09-0.21567100E-  
 13 2  
 0.25667661E+05-0.28003713E+01 0.20135620E+01 0.15190450E-01-0.16163190E-  
 04 3  
 0.90789920E-08-0.19127460E-11 0.26124440E+05 0.88053780E+01  
 4  
 C2H4Z C 2H 4O 0 G 0300.00 5000.00 1090.00  
 1  
 0.31468137E+00 0.16729900E-01-0.68090900E-05 0.12292200E-08-0.82392800E-  
 13 2

0.57249924E+04 0.20362720E+02 0.13181000E+01 0.14446000E-01-0.27433500E-  
 05 3  
 -0.31083500E-08 0.15277200E-11 0.52681700E+04 0.14723300E+02  
 4  
 C2H6 C 2H 6O 0 G 0300.00 5000.00 1250.00  
 1  
 0.31208901E+00 0.21192800E-01-0.80856000E-05 0.13933900E-08-0.90300500E-  
 13 2  
 -0.10989168E+05 0.20203763E+02 0.97545400E+00 0.18811000E-01-0.14645300E-  
 05 3  
 -0.63824700E-08 0.28406700E-11-0.11311100E+05 0.16551400E+02  
 4  
 CH2COZ C 2H 2O 1 G 0300.00 5000.00 1000.00  
 1  
 0.53510982E+01 0.69420900E-02-0.25006100E-05 0.41323100E-09-0.25969200E-  
 13 2  
 -0.78085131E+04-0.37920071E+01 0.29953900E+01 0.12354000E-01-0.40649900E-  
 05 3  
 -0.33460800E-08 0.22415200E-11-0.71509700E+04 0.85371600E+01  
 4  
 CH3CHO C 2H 4O 1 G 0300.00 5000.00 1000.00  
 1  
 0.42598131E+01 0.13486034E-01-0.49183418E-05 0.82515045E-09-0.52694343E-  
 13 2  
 -0.22171378E+05 0.29348441E+01 0.26969113E+01 0.12334284E-01 0.56746453E-  
 05 3  
 -0.10870704E-07 0.37648248E-11-0.21403137E+05 0.12530482E+02  
 4  
 C2H5OH C 2H 6O 1 G 0300.00 5000.00 1000.00  
 1  
 0.56164566E+01 0.15991600E-01-0.53679900E-05 0.84342200E-09-0.51140600E-  
 13 2  
 -0.31041092E+05-0.35594342E+01 0.93985800E+00 0.26181100E-01-0.92513400E-  
 05 3  
 -0.34582500E-08 0.26209800E-11-0.29623800E+05 0.21263400E+02  
 4  
 C2H5OOH C 2H 6O 2 G 0300.00 5000.00 1000.00  
 1  
 0.88514772E+01 0.14699100E-01-0.46663000E-05 0.70312900E-09-0.41326200E-  
 13 2  
 -0.23452357E+05-0.17367764E+02 0.20326600E+01 0.32031000E-01-0.17977300E-  
 04 3  
 0.23876600E-08 0.10720600E-11-0.21506300E+05 0.18218700E+02  
 4  
 CH3COOH C 2H 4O 3 G 0300.00 5000.00 1000.00  
 1  
 0.78670144E+01 0.14240000E-01-0.48164800E-05 0.76239600E-09-0.46551400E-  
 13 2  
 -0.43975651E+05-0.96455346E+01 0.21956900E+00 0.35313100E-01-0.22427600E-  
 04 3  
 0.32288800E-08 0.16724300E-11-0.41954800E+05 0.29661700E+02  
 4  
 ! Ajout produits en C2+  
 !C3H4 OC 3H 4 G 0300.00 5000.00  
 1000.00  
 ! .54693928E+01 .12151568E-01 -.43443515E-05 .71433565E-09 -.44747395E-  
 13

! .19852377E+05 -.54474335E+01 .22271647E+01 .19307628E-01 -.70081351E-05  
 !-.27282026E-08 .21393857E-11 .20828311E+05 .11726395E+02  
 C3H6Y OC 3H 6 G 0300.00 5000.00 1000.00  
 1  
 0.49872203E+01 0.17638993E-01-0.62266308E-05 0.10151433E-08-0.63235977E-13  
 2  
 -0.25513278E+03-0.23657645E+01 0.55598283E+00 0.27091531E-01-0.10752104E-04  
 3  
 -0.97539210E-09 0.14314721E-11 0.11570190E+04 0.21344173E+02  
 4  
 C3H8 OC 3H 8 G 0300.00 5000.00 1000.00  
 1  
 0.54507892E+01 0.22160569E-01-0.77296281E-05 0.12495476E-08-0.77377605E-13  
 2  
 -0.15616278E+05-0.61404570E+01-0.31831896E+00 0.34746405E-01-0.12885018E-04  
 3  
 -0.35057037E-08 0.30165358E-11-0.13851594E+05 0.24514595E+02  
 4  
 C4H6Z2-13 OC 4H 6 G 0300.00 5000.00 1000.00  
 1  
 0.80531918E+01 0.17540889E-01-0.61760657E-05 0.10047656E-08-0.62479542E-13  
 2  
 0.95684505E+04-0.18621006E+02-0.29224473E+00 0.38725201E-01-0.16706719E-04  
 3  
 -0.81080902E-08 0.67421541E-11 0.11749236E+05 0.24444702E+02  
 4  
 nC4H8Y OC 4H 8 G 0300.00 5000.00 1000.00  
 1  
 0.92846959E+01 0.19871462E-01-0.65713975E-05 0.10258888E-08-0.62160394E-13  
 2  
 -0.46494721E+04-0.24153239E+02-0.25869742E+00 0.41475497E-01-0.21317686E-04  
 3  
 0.27918821E-08 0.85749311E-12-0.16180958E+04 0.26720718E+02  
 4  
 C4H10 OC 4H 10 G 0300.00 5000.00 1000.00  
 1  
 0.76947071E+01 0.27767614E-01-0.96156327E-05 0.15456056E-08-0.95281279E-13  
 2  
 -0.19406615E+05-0.16133800E+02 0.59979584E-01 0.44005580E-01-0.15532127E-04  
 3  
 -0.52806315E-08 0.40442116E-11-0.17040045E+05 0.24565849E+02  
 4  
 C2H3CHOZ OC 3H 4O 1 G 0300.00 5000.00 1000.00  
 1  
 0.12217825E+02 0.12961588E-01-0.61774654E-05 0.12501405E-08-0.91169971E-13  
 2  
 -0.15124886E+05-0.41653439E+02 0.93137437E+00 0.35574418E-01-0.33347264E-04  
 3  
 0.28398034E-07-0.11395644E-10-0.10614329E+05 0.21059492E+02  
 4  
 C2H5CHO OC 3H 6O 1 G 0300.00 5000.00 1000.00  
 1  
 0.69979400E+01 0.18013448E-01-0.62295217E-05 0.10005839E-08-0.61661722E-13  
 2  
 -0.25678625E+05-0.94601873E+01 0.28277023E+01 0.25430365E-01-0.61913220E-05  
 3

-0.50245177E-08 0.26785609E-11-0.24271348E+05 0.13234089E+02  
 4  
 C3H7OH 0C 3H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.71550135E+01 0.22466624E-01-0.76292372E-05 0.12097231E-08-0.73884075E-  
 13 2  
 -0.34674318E+05-0.94533208E+01 0.12350693E+01 0.34453284E-01-0.10589133E-  
 04 3  
 -0.54856804E-08 0.35146994E-11-0.32804938E+05 0.22268148E+02  
 4  
 C2H6CO 0C 3H 60 1 G 0300.00 5000.00 1000.00  
 1  
 0.59760364E+01 0.19679097E-01-0.70154574E-05 0.11513579E-08-0.72035416E-  
 13 2  
 -0.29341092E+05-0.53765277E+01 0.14577827E+01 0.28063715E-01-0.90218518E-  
 05 3  
 -0.24536706E-08 0.16730232E-11-0.27794104E+05 0.19218454E+02  
 4  
 C3H8CO 0C 4H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.87691958E+01 0.24174010E-01-0.83446403E-05 0.13376648E-08-0.82271822E-  
 13 2  
 -0.32998668E+05-0.17683410E+02 0.27316518E+01 0.35815358E-01-0.11085016E-  
 04 3  
 -0.44516226E-08 0.28435873E-11-0.31006189E+05 0.14949604E+02  
 4  
 R1H C 0H 10 0 G 0300.00 5000.00 1000.00  
 1  
 0.25138341E+01 0.40918900E-05-0.24108200E-08 0.57187400E-12-0.47091700E-  
 16 2  
 0.25465395E+05-0.53483352E+00 0.25198400E+01-0.25992000E-04 0.62789800E-  
 07 3  
 -0.62995100E-10 0.22397300E-13 0.25464100E+05-0.56325900E+00  
 4  
 R2OH C 0H 10 1 G 0300.00 5000.00 1000.00  
 1  
 0.30414122E+01 0.65138500E-03-0.19121800E-07-0.10419600E-12 0.40033000E-  
 16 2  
 0.39041469E+04 0.48177896E+01 0.36778000E+01-0.21415300E-03 0.57023100E-  
 07 3  
 0.17140400E-09-0.18462900E-13 0.36359700E+04 0.11967000E+01  
 4  
 R3OOH C 0H 10 2 G 0300.00 5000.00 1000.00  
 1  
 0.47320384E+01 0.13862200E-02-0.16845700E-06 0.10584300E-10-0.24071700E-  
 15 2  
 -0.25323960E+03-0.76677917E+00 0.18485400E+01 0.10798800E-01-0.85463500E-  
 05 3  
 0.41841500E-09 0.14407400E-11 0.32644600E+03 0.13431900E+02  
 4  
 R4CH3 C 1H 30 0 G 0300.00 5000.00 1022.00  
 1  
 0.29723911E+01 0.62323902E-02-0.22190404E-05 0.36577827E-09-0.23059057E-  
 13 2  
 0.15991251E+05 0.43951618E+01 0.30266473E+01 0.45351572E-02 0.68535263E-  
 06 3  
 -0.10839243E-08 0.15497636E-12 0.16144411E+05 0.47042460E+01  
 4

R5CHO C 1H 10 1 G 0300.00 5000.00 1000.00  
1  
0.36073098E+01 0.28745262E-02-0.98788814E-06 0.15840323E-09-0.97735176E-  
14 2  
0.32342028E+04 0.54449718E+01 0.35340273E+01 0.20234731E-02 0.51834081E-  
06 3  
-0.37246076E-09-0.60802857E-13 0.33738574E+04 0.62388401E+01  
4  
R6CH2OH C 1H 30 1 G 0300.00 5000.00 1000.00  
1  
0.59488653E+01 0.36190501E-02-0.61752752E-06 0.59083634E-10-0.25698620E-  
14 2  
-0.36338402E+04-0.62813047E+01 0.21966424E+01 0.12963202E-01-0.12844380E-  
04 3  
0.99145598E-08-0.32231225E-11-0.22978342E+04 0.13927387E+02  
4  
R7CH3O C 1H 30 1 G 0300.00 5000.00 1000.00  
1  
0.64455491E+01 0.32218200E-02-0.50980100E-06 0.44196600E-10-0.16936600E-  
14 2  
-0.81072981E+03-0.12161207E+02 0.24057100E+00 0.18774700E-01-0.21318000E-  
04 3  
0.18115100E-07-0.66123000E-11 0.13582700E+04 0.21181500E+02  
4  
R8CH3OO C 1H 30 2 G 0300.00 5000.00 1000.00  
1  
0.97570050E+01 0.30427600E-02-0.46705400E-06 0.38783300E-10-0.13942500E-  
14 2  
-0.19046129E+04-0.26874937E+02 0.14893700E+01 0.24077600E-01-0.23874800E-  
04 3  
0.15153500E-07-0.44755700E-11 0.76434000E+03 0.16985200E+02  
4  
R9C2HT C 2H 10 0 G 0300.00 5000.00 1000.00  
1  
0.40394303E+01 0.36123355E-02-0.95946029E-06 0.12793372E-09-0.69526612E-  
14 2  
0.65952283E+05 0.20001883E+01 0.17718196E+01 0.17070146E-01-0.20073590E-  
04 3  
0.88779526E-08-0.83304159E-12 0.65840078E+05 0.11053392E+02  
4  
R10C2H3V C 2H 30 0 G 0300.00 5000.00 1000.00  
1  
0.50727923E+01 0.54012556E-02-0.12119358E-05 0.14271406E-09-0.71272656E-  
14 2  
0.33707740E+05-0.30985539E+01 0.12316554E+01 0.14659354E-01-0.95136020E-  
05 3  
0.36466949E-08-0.62640339E-12 0.34934910E+05 0.17314640E+02  
4  
R11C2H5 C 2H 50 0 G 0300.00 5000.00 1000.00  
1  
0.35019849E+01 0.12614300E-01-0.36573000E-05 0.51664200E-09-0.29046900E-  
13 2  
0.12403884E+05 0.54466514E+01 0.54658000E+00 0.20436800E-01-0.11669400E-  
04 3  
0.48254100E-08-0.11928100E-11 0.13274300E+05 0.20900100E+02  
4  
R12CHCOV C 2H 10 1 G 0300.00 5000.00 1000.00  
1



0.67580728E+01 0.20004000E-02-0.20276070E-06-0.10411320E-09 0.19651650E-  
 13 2  
 0.19015137E+05-0.90712611E+01 0.50479650E+01 0.44534780E-02 0.22682830E-  
 06 3  
 -0.14820950E-08 0.22507420E-12 0.19658920E+05 0.48184390E+00  
 4  
 R13CH2CHO C 2H 3O 1 G 0300.00 5000.00 1000.00  
 1  
 0.92088690E+01 0.36510697E-02-0.64394158E-06 0.63296798E-10-0.28066517E-  
 14 2  
 -0.71802166E+03-0.24495662E+02 0.13357744E+01 0.22153886E-01-0.20867239E-  
 04 3  
 0.14634303E-07-0.49802371E-11 0.19974985E+04 0.17885937E+02  
 4  
 R14CH3CO C 2H 3O 1 G 0300.00 5000.00 1000.00  
 1  
 0.10949532E+02 0.54414349E-03-0.15865876E-07-0.23107392E-12 0.46252823E-  
 16 2  
 -0.60857281E+04-0.33427422E+02 0.38579266E+01 0.54023149E-02 0.94996667E-  
 05 3  
 -0.93490025E-08 0.20667194E-11-0.26711941E+04 0.85433064E+01  
 4  
 R15C2H5O C 2H 5O 1 G 0300.00 5000.00 1000.00  
 1  
 0.87906851E+01 0.83791700E-02-0.19344600E-05 0.22937100E-09-0.11319100E-  
 13 2  
 -0.60285190E+04-0.22314638E+02-0.60009300E+00 0.31767000E-01-0.24258600E-  
 04 3  
 0.10813700E-07-0.22685600E-11-0.30849100E+04 0.27365000E+02  
 4  
 R16C2H4OOH C 2H 5O 2 G 0300.00 5000.00 1000.00  
 1  
 0.98523206E+01 0.10040573E-01-0.24779133E-05 0.31358741E-09-0.16472921E-  
 13 2  
 0.79572587E+03-0.20532601E+02 0.11050612E+01 0.41490670E-01-0.47184953E-  
 04 3  
 0.30393178E-07-0.80918614E-11 0.28154634E+04 0.22787066E+02  
 4  
 R17C2H5OO C 2H 5O 2 G 0300.00 5000.00 1000.00  
 1  
 0.11317384E+02 0.82862500E-02-0.18620300E-05 0.21820900E-09-0.10786800E-  
 13 2  
 -0.69786387E+04-0.32893885E+02 0.67205600E+00 0.36275700E-01-0.30000800E-  
 04 3  
 0.13847900E-07-0.28458300E-11-0.37888600E+04 0.22886900E+02  
 4  
 R18CH3COOO C 2H 3O 3 G 0300.00 5000.00 1000.00  
 1  
 0.58289108E+01 0.14517937E-01-0.45853781E-05 0.69238965E-09-0.40972888E-  
 13 2  
 -0.24628644E+05 0.41316311E+00-0.10923432E+01 0.39162144E-01-0.33321889E-  
 04 3  
 0.13345456E-07-0.16804813E-11-0.23286021E+05 0.34139729E+02  
 4  
 R19C3H7 C 3H 7O 0 G 0300.00 5000.00 1000.00  
 1  
 0.49242144E+01 0.19549200E-01-0.60986200E-05 0.90898600E-09-0.53099400E-  
 13 2

0.97114243E+04 0.13299184E+00-0.99704900E+00 0.42263700E-01-0.36768300E-  
 04 3  
 0.18398500E-07-0.36661700E-11 0.10848900E+05 0.28729400E+02  
 4  
 R20C4H9 C 4H 90 0 G 0300.00 5000.00 1000.00  
 1  
 0.70528222E+01 0.25322100E-01-0.80453100E-05 0.12138300E-08-0.71451200E-  
 13 2  
 0.55184302E+04-0.91858723E+01-0.50611900E+00 0.50722100E-01-0.37439800E-  
 04 3  
 0.14596600E-07-0.19007900E-11 0.71957100E+04 0.28323100E+02  
 4  
 R21CH3OCO C 2H 30 2 G 0300.00 5000.00 1000.00  
 1  
 0.93943954E+01 0.74243200E-02-0.26564100E-05 0.42503100E-09-0.25182400E-  
 13 2  
 -0.23221392E+05-0.21236261E+02 0.41621500E+01 0.13803700E-01-0.30848600E-  
 06 3  
 -0.45643000E-08 0.14690900E-11-0.21013000E+05 0.86430100E+01  
 4  
 R22CO2H C 1H 10 2 G 0300.00 5000.00 1000.00  
 1  
 0.28866306E+01 0.68517160E-02 0.10166207E-05-0.48945155E-08 0.20869597E-  
 11 2  
 -0.24362560E+05 0.12138004E+02 0.52000489E+01 0.33457270E-02-0.66695446E-  
 06 3  
 0.71988131E-10-0.33980889E-14-0.25185346E+05-0.62765884E+00  
 4  
 R23C2H3O2B C 2H 30 2 G 0300.00 5000.00 1000.00  
 1  
 0.93245482E+01 0.69435383E-02-0.16960130E-05 0.21230508E-09-0.11030391E-  
 13 2  
 -0.33662305E+05-0.23251428E+02 0.18895344E+00 0.34251921E-01-0.33446948E-  
 04 3  
 0.17838767E-07-0.40593453E-11-0.31194209E+05 0.23558701E+02  
 4  
 R24C2H4OH T 4/83 C 2H 50 10 OG 300.00 5000.0 1000.00  
 1  
 0.75944829E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-  
 13 2  
 -0.57728535E+04-0.13969286E+02 0.14019508E+01 0.21543175E-01-0.22326512E-  
 05 3  
 -0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19135818E+02  
 4  
 R25C2H4OH T 4/83 C 2O 1H 5 OG 300.000 5000.00 1000.0  
 1  
 0.67665967E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-  
 13 2  
 -0.56093438E+04-0.93984114E+01 0.24813328E+01 0.16790036E-01 0.37755499E-  
 05 3  
 -0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02  
 4  
 C2H4OE#3 C 2H 40 1 G 0300.00 5000.00 1000.00  
 1  
 0.43068863E+01 0.13877206E-01-0.51784232E-05 0.88229646E-09-0.56921298E-  
 13 2  
 -0.86772809E+04-0.38457474E+00-0.92033523E+00 0.26421962E-01-0.13407433E-  
 04 3

0.31399369E-09 0.14228568E-11-0.71333140E+04 0.27113031E+02  
 4  
 C5H12-1 C 5H 120 0 G 0300.00 5000.00 1000.00  
 1  
 0.54709163E+01 0.40745795E-01-0.15107792E-04 0.25635050E-08-0.16496268E-  
 12 2  
 -0.21177338E+05-0.14309943E+01 0.91293097E-01 0.53016998E-01-0.13679948E-  
 04 3  
 -0.14501379E-07 0.85804974E-11-0.19892135E+05 0.26246931E+02  
 4  
 C6H12OA-1 C 6H 120 1 G 0300.00 5000.00 1000.00  
 1  
 0.12807075E+02 0.36472440E-01-0.12767808E-04 0.20821860E-08-0.13042619E-  
 12 2  
 -0.36247336E+05-0.34741486E+02 0.19369314E+01 0.60015842E-01-0.20683741E-  
 04 3  
 -0.95685619E-08 0.67629955E-11-0.32976250E+05 0.22921597E+02  
 4  
 C6H12O2B-1 C 6H 120 2 G 0300.00 5000.00 1000.00  
 1  
 0.15211798E+02 0.36151856E-01-0.12438441E-04 0.20018232E-08-0.12413986E-  
 12 2  
 -0.68083523E+05-0.46625908E+02-0.16093326E+01 0.88164434E-01-0.70082919E-  
 04 3  
 0.27866587E-07-0.35358745E-11-0.63837703E+05 0.38611351E+02  
 4  
 C4H8OA C 4H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.78373337E+01 0.25887879E-01-0.92356704E-05 0.15248637E-08-0.96257942E-  
 13 2  
 -0.29861789E+05-0.13612039E+02-0.19119226E+01 0.52698199E-01-0.32785865E-  
 04 3  
 0.67593700E-08 0.11583668E-11-0.27227180E+05 0.36639725E+02  
 4  
 C5H10OA C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C5H10OK C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C6H10O2A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4

C6H1002KA                    C    6H   100   2            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C6H1003AB                    C    6H   100   3            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C6H1003KB                    C    6H   100   3            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C3H603KP                    C    3H    60   3            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C4H803KP                    C    4H    80   3            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C5H1003KP                    C    5H   100   3            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C6H1004KAP                    C    6H   100   4            G   0300.00    5000.00    1000.00  
1  
0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
12        2  
-0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
04        3  
0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
4  
C6H1005KPB                    C    6H   100   5            G   0300.00    5000.00    1000.00  
1

0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C4H6O4KAP C 4H 60 4 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C3H4O4KAP C 3H 40 4 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C4H6O5KPB C 4H 60 5 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 C3H4O5KPB C 3H 40 5 G 0300.00 5000.00 1000.00  
 1  
 0.10793698E+02 0.30298827E-01-0.10570229E-04 0.17185927E-08-0.10737029E-  
 12 2  
 -0.32946293E+05-0.25868876E+02 0.54039097E+00 0.58913231E-01-0.38187045E-  
 04 3  
 0.11537297E-07-0.67035564E-12-0.30136662E+05 0.27020313E+02  
 4  
 M31C5H10Y C 5H 100 0 G 0300.00 5000.00 1000.00  
 1  
 0.64338064E+01 0.33465367E-01-0.12206403E-04 0.20472852E-08-0.13067345E-  
 12 2  
 -0.75642852E+04-0.61613674E+01 0.97608697E+00 0.44395778E-01-0.10314980E-  
 04 3  
 -0.12274562E-07 0.68270580E-11-0.60133306E+04 0.22697617E+02  
 4  
 M32C5H10Z C 5H 100 0 G 0300.00 5000.00 1000.00  
 1  
 0.68866458E+01 0.33219494E-01-0.12162192E-04 0.20454378E-08-0.13081308E-  
 12 2  
 -0.64481338E+04-0.83398561E+01 0.19331774E+00 0.48487734E-01-0.15268532E-  
 04 3  
 -0.10284795E-07 0.67308472E-11-0.46432534E+04 0.26575609E+02  
 4  
 M38C6H10OAZ C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.89591398E+01 0.41732229E-01-0.16714626E-04 0.29922591E-08-0.19984143E-  
 12 2

-0.22713266E+05-0.15889680E+02-0.28324190E+00 0.59067763E-01-0.22940723E-  
 04 3  
 -0.13757750E-08 0.23011371E-11-0.19471473E+05 0.34562714E+02  
 4  
 M35C6H10OAZ C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.11548041E+02 0.33124030E-01-0.11782113E-04 0.19414199E-08-0.12239347E-  
 12 2  
 -0.21654615E+05-0.27799288E+02 0.11371523E+01 0.55758715E-01-0.19454008E-  
 04 3  
 -0.93345864E-08 0.66017118E-11-0.18529590E+05 0.27395493E+02  
 4  
 M34C6H10OAZ C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.12088802E+02 0.31860996E-01-0.11134631E-04 0.18125116E-08-0.11332827E-  
 12 2  
 -0.22291080E+05-0.30765463E+02 0.30584595E+01 0.50563488E-01-0.16504820E-  
 04 3  
 -0.78361451E-08 0.52333689E-11-0.19479096E+05 0.17476084E+02  
 4  
 M33C6H10OAZ C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.12548502E+02 0.31467892E-01-0.11002681E-04 0.17915970E-08-0.11204048E-  
 12 2  
 -0.21047797E+05-0.32931522E+02 0.10713750E+01 0.61664551E-01-0.35455028E-  
 04 3  
 0.54654294E-08 0.19469415E-11-0.17848471E+05 0.26639822E+02  
 4  
 C5H8OAZ C 5H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.10605665E+02 0.25413850E-01-0.88880897E-05 0.14463630E-08-0.90349955E-  
 13 2  
 -0.17569977E+05-0.24479416E+02 0.10031602E+01 0.51833943E-01-0.33518820E-  
 04 3  
 0.93631796E-08-0.19402329E-12-0.14925744E+05 0.25134592E+02  
 4  
 C4H6OAZ C 4H 60 1 G 0300.00 5000.00 1000.00  
 1  
 0.56204925E+01 0.28762365E-01-0.12229204E-04 0.22837559E-08-0.15720068E-  
 12 2  
 -0.15934229E+05-0.19152337E+01 0.22208357E+01 0.25523838E-01 0.68321147E-  
 05 3  
 -0.14445181E-07 0.41486016E-11-0.13948009E+05 0.19776493E+02  
 4  
 M39C6H10OKZ C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.11090804E+02 0.25835335E-01-0.75559028E-05 0.10855972E-08-0.62387412E-  
 13 2  
 -0.13617819E+05-0.40710556E+02 0.10065230E-01 0.49785316E-01-0.15109136E-  
 04 3  
 -0.11719950E-07 0.74271518E-11-0.10290848E+05 0.18055246E+02  
 4  
 M45C6H10O2ZB C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.13361590E+02 0.32559805E-01-0.11186725E-04 0.17996302E-08-0.11162482E-  
 12 2  
 -0.53807082E+05-0.36025707E+02-0.64123052E+00 0.75208656E-01-0.56723198E-  
 04 3

0.20398556E-07-0.18201083E-11-0.50257898E+05 0.35049217E+02  
 4  
 M42C6H1002ZB C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.13813983E+02 0.33227529E-01-0.11666058E-04 0.19032560E-08-0.11908061E-  
 12 2  
 -0.53213469E+05-0.38902958E+02 0.57423574E+00 0.63947283E-01-0.23248802E-  
 04 3  
 -0.14207145E-07 0.10094058E-10-0.49487711E+05 0.30442446E+02  
 4  
 M41C6H1002ZB C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.14456921E+02 0.31847406E-01-0.10996652E-04 0.17759082E-08-0.11048272E-  
 12 2  
 -0.53907305E+05-0.42472603E+02 0.10810851E+01 0.68314567E-01-0.42452564E-  
 04 3  
 0.83854559E-08 0.16445565E-11-0.50283137E+05 0.26543251E+02  
 4  
 M40C6H1002ZB C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.14930683E+02 0.31436045E-01-0.10855283E-04 0.17530372E-08-0.10905303E-  
 12 2  
 -0.52671316E+05-0.44720863E+02-0.10641770E+01 0.80520347E-01-0.64074768E-  
 04 3  
 0.24371092E-07-0.25970654E-11-0.48635691E+05 0.36375809E+02  
 4  
 C5H8O2ZB C 5H 80 2 G 0300.00 5000.00 1000.00  
 1  
 0.12950788E+02 0.25439052E-01-0.87725157E-05 0.14150188E-08-0.87935539E-  
 13 2  
 -0.49176516E+05-0.36057434E+02-0.86289656E+00 0.68825014E-01-0.57670113E-  
 04 3  
 0.23818941E-07-0.31665378E-11-0.45741871E+05 0.33728638E+02  
 4  
 C4H6O2ZB C 4H 60 2 G 0300.00 5000.00 1000.00  
 1  
 0.93207579E+01 0.20578479E-01-0.70078099E-05 0.11193776E-08-0.69041317E-  
 13 2  
 -0.46724883E+05-0.18044838E+02 0.17438633E+01 0.42412765E-01-0.28511282E-  
 04 3  
 0.86043359E-08-0.30791881E-12-0.44720773E+05 0.20776680E+02  
 4  
 C3H4O2ZB C 3H 40 2 G 0300.00 5000.00 1000.00  
 1  
 0.79218497E+01 0.15470609E-01-0.55981855E-05 0.93352825E-09-0.59335756E-  
 13 2  
 -0.43954641E+05-0.12798262E+02 0.12327962E+01 0.31435639E-01-0.12333403E-  
 04 3  
 -0.67854873E-08 0.51189213E-11-0.42108926E+05 0.22089104E+02  
 4  
 C5H12O2P C 5H 120 2 G 0300.00 5000.00 1000.00  
 1  
 0.14755652E+02 0.33111449E-01-0.11136997E-04 0.17624443E-08-0.10795160E-  
 12 2  
 -0.37013109E+05-0.43265808E+02 0.60896840E+01 0.35711069E-01 0.40240484E-  
 04 3  
 -0.73305458E-07 0.29648818E-10-0.33957156E+05 0.58916650E+01  
 4

C6H12O3AP                    C    6H   12O    3            G   0300.00    5000.00    1000.00  
1  
0.18682959E+02 0.34876753E-01-0.11780321E-04 0.18720125E-08-0.11511086E-  
12        2  
-0.50079445E+05-0.58733673E+02 0.74818194E+00 0.85583627E-01-0.58291669E-  
04        3  
0.14156047E-07 0.13401045E-11-0.45356375E+05 0.33245693E+02  
4  
C6H12O4PB                    C    6H   12O    4            G   0300.00    5000.00    1000.00  
1  
0.20627451E+02 0.35495616E-01-0.11926038E-04 0.18895194E-08-0.11602378E-  
12        2  
-0.81491797E+05-0.68707909E+02 0.24213197E+01 0.78615047E-01-0.26847745E-  
04        3  
-0.24421947E-07 0.16203851E-10-0.76557586E+05 0.26087534E+02  
4  
C3H6O2PZ                    C    3H    6O    2            G   0300.00    5000.00    1000.00  
1  
0.10443696E+02 0.17573746E-01-0.60961356E-05 0.98704911E-09-0.61481954E-  
13        2  
-0.11948630E+05-0.24820234E+02 0.36786113E+01 0.32269310E-01-0.10301906E-  
04        3  
-0.76882758E-08 0.48891334E-11-0.99506963E+04 0.10972757E+02  
4  
C4H8O2PZ                    C    4H    8O    2            G   0300.00    5000.00    1000.00  
1  
0.13172652E+02 0.21643989E-01-0.71929812E-05 0.11303418E-08-0.68989261E-  
13        2  
-0.17775795E+05-0.36529381E+02 0.22901256E+01 0.47590896E-01-0.18961156E-  
04        3  
-0.95546548E-08 0.73198019E-11-0.14750507E+05 0.20296099E+02  
4  
C5H10O2PZ                    C    5H   10O    2            G   0300.00    5000.00    1000.00  
1  
0.14148792E+02 0.30025356E-01-0.10455547E-04 0.16959014E-08-0.10567980E-  
12        2  
-0.18861838E+05-0.40862545E+02 0.46716652E+01 0.42237498E-01 0.14331417E-  
04        3  
-0.46159837E-07 0.20228080E-10-0.15855921E+05 0.10865979E+02  
4  
C5H8O3APZ                    C    5H    8O    3            G   0300.00    5000.00    1000.00  
1  
0.16490452E+02 0.24039069E-01-0.80427108E-05 0.12684102E-08-0.77529061E-  
13        2  
-0.31198455E+05-0.48543991E+02 0.14703654E+01 0.66393606E-01-0.46193098E-  
04        3  
0.10381412E-07 0.16254048E-11-0.27257680E+05 0.28468348E+02  
4  
C4H6O3APZ                    C    4H    6O    3            G   0300.00    5000.00    1000.00  
1  
0.14991622E+02 0.16342105E-01-0.50932613E-05 0.76430134E-09-0.45168178E-  
13        2  
-0.27547982E+05-0.42445545E+02 0.56280761E+01 0.31040274E-01 0.52769033E-  
05        3  
-0.26281787E-07 0.11296134E-10-0.24496980E+05 0.85323267E+01  
4  
C3H4O3APZ                    C    3H    4O    3            G   0300.00    5000.00    1000.00  
1



0.10257364E+02 0.21121712E-01-0.93092422E-05 0.17832507E-08-0.12501657E-  
 12 2  
 -0.23205748E+05-0.21822023E+02 0.13224814E+01 0.42937476E-01-0.32259974E-  
 04 3  
 0.15829880E-07-0.41017953E-11-0.20244805E+05 0.25869549E+02  
 4  
 C6H10O3KPZ C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.18565212E+02 0.21948731E-01-0.58204801E-05 0.77917989E-09-0.42675461E-  
 13 2  
 -0.27902070E+05-0.73297005E+02 0.20636480E+01 0.59524477E-01-0.22776432E-  
 04 3  
 -0.12725216E-07 0.93434913E-11-0.23037529E+05 0.13748915E+02  
 4  
 C5H8O4PZB C 5H 80 4 G 0300.00 5000.00 1000.00  
 1  
 0.18514725E+02 0.24542632E-01-0.81357412E-05 0.12755866E-08-0.77698671E-  
 13 2  
 -0.62649461E+05-0.58976944E+02 0.24705014E+01 0.64026244E-01-0.25574422E-  
 04 3  
 -0.17680911E-07 0.12878091E-10-0.58386184E+05 0.24168240E+02  
 4  
 C4H6O4PZB C 4H 60 4 G 0300.00 5000.00 1000.00  
 1  
 0.17427374E+02 0.16245307E-01-0.49426089E-05 0.72852718E-09-0.42499397E-  
 13 2  
 -0.59194777E+05-0.55236755E+02 0.37463241E+01 0.48139583E-01-0.19137186E-  
 04 3  
 -0.11555581E-07 0.82229588E-11-0.55311406E+05 0.16499939E+02  
 4  
 C3H4O4PZB C 3H 40 4 G 0300.00 5000.00 1000.00  
 1  
 0.13377137E+02 0.13896868E-01-0.45495158E-05 0.70759876E-09-0.42893715E-  
 13 2  
 -0.53762812E+05-0.35391850E+02 0.10392102E+01 0.58437455E-01-0.64131156E-  
 04 3  
 0.35253819E-07-0.72101344E-11-0.51037742E+05 0.25362167E+02  
 4  
 C4H6O2A2 C 4H 60 2 G 0300.00 5000.00 1000.00  
 1  
 0.10464355E+02 0.19915162E-01-0.68624568E-05 0.11055530E-08-0.68604593E-  
 13 2  
 -0.39741125E+05-0.22447149E+02 0.19222121E+01 0.47891930E-01-0.43315311E-  
 04 3  
 0.23579142E-07-0.55239645E-11-0.37563738E+05 0.20682190E+02  
 4  
 C3H4O2A2 C 3H 40 2 G 0300.00 5000.00 1000.00  
 1  
 0.65950022E+01 0.17324423E-01-0.64571268E-05 0.10998213E-08-0.70970438E-  
 13 2  
 -0.36926754E+05-0.32180970E+01-0.68121254E-01 0.38418576E-01-0.32508411E-  
 04 3  
 0.15964680E-07-0.33155742E-11-0.35194238E+05 0.30596817E+02  
 4  
 C4H6O3KPZ C 4H 60 3 G 0300.00 5000.00 1000.00  
 1  
 0.13981548E+02 0.11268719E-01-0.25222571E-05 0.29860256E-09-0.15084124E-  
 13 2

-0.20975389E+05-0.52602669E+02 0.20329032E+01 0.39066538E-01-0.16788392E-  
 04 3  
 -0.72867663E-08 0.59872454E-11-0.17474398E+05 0.10298769E+02  
 4  
 C3H4O3KPZ C 3H 4O 3 G 0300.00 5000.00 1000.00  
 1  
 0.10878807E+02 0.68324399E-02-0.12816249E-05 0.13238290E-09-0.60834406E-  
 14 2  
 -0.14573443E+05-0.37945984E+02 0.59226584E+00 0.35476360E-01-0.29318264E-  
 04 3  
 0.10783248E-07-0.97768907E-12-0.11731711E+05 0.15177939E+02  
 4  
 C4H6O3AB C 4H 6O 3 G 0300.00 5000.00 1000.00  
 1  
 0.12842388E+02 0.19894594E-01-0.67265287E-05 0.10701644E-08-0.65884371E-  
 13 2  
 -0.71363172E+05-0.33521629E+02-0.14141127E+00 0.66252433E-01-0.70754904E-  
 04 3  
 0.41316842E-07-0.96582247E-11-0.68358703E+05 0.30806156E+02  
 4  
 C3H4O3AB C 3H 4O 3 G 0300.00 5000.00 1000.00  
 1  
 0.89766827E+01 0.17253103E-01-0.62592953E-05 0.10456614E-08-0.66546771E-  
 13 2  
 -0.68543633E+05-0.14292747E+02-0.20116405E+01 0.55929273E-01-0.57861424E-  
 04 3  
 0.31571588E-07-0.66781923E-11-0.66001836E+05 0.40214397E+02  
 4  
 C3H4OKZ C 3H 4O 1 G 0300.00 5000.00 1000.00  
 1  
 0.34068933E+01 0.10705855E-01-0.27336589E-05 0.35526754E-09-0.19031782E-  
 13 2  
 -0.23973071E+04-0.48015146E+01 0.10790132E+01 0.15444501E-01-0.36694137E-  
 05 3  
 -0.24154410E-08 0.12766650E-11-0.16932944E+04 0.76077871E+01  
 4  
 C4H6OKZ C 4H 6O 1 G 0300.00 5000.00 1000.00  
 1  
 0.50813050E+01 0.17146232E-01-0.49012046E-05 0.69313777E-09-0.39430441E-  
 13 2  
 -0.57959985E+04-0.11864973E+02 0.16615275E+00 0.27908828E-01-0.53418121E-  
 05 3  
 -0.10495363E-07 0.57422335E-11-0.44744829E+04 0.13829488E+02  
 4  
 C3H8OL C 3H 8O 1 G 0300.00 5000.00 1000.00  
 1  
 0.78738937E+01 0.22170236E-01-0.76477927E-05 0.12332934E-08-0.76598667E-  
 13 2  
 -0.36674129E+05-0.15277677E+02 0.13337798E+00 0.40273454E-01-0.14728696E-  
 04 3  
 -0.80114964E-08 0.58863921E-11-0.34506324E+05 0.25219995E+02  
 4  
 C3H8O2P C 3H 8O 2 G 0300.00 5000.00 1000.00  
 1  
 0.10592219E+02 0.21092908E-01-0.69577177E-05 0.10872773E-08-0.66088445E-  
 13 2  
 -0.27541844E+05-0.24401106E+02 0.18213568E+01 0.42758811E-01-0.20479554E-  
 04 3

-0.19162016E-08 0.35641871E-11-0.25071838E+05 0.21374474E+02  
 4  
 C4H10 C 4H 100 0 G 0300.00 5000.00 1000.00  
 1  
 0.39652297E+01 0.34151986E-01-0.12778572E-04 0.21821218E-08-0.14104363E-  
 12 2  
 -0.18969699E+05 0.24376407E+01-0.20567587E+00 0.44319719E-01-0.13659372E-  
 04 3  
 -0.88613223E-08 0.57863727E-11-0.18013684E+05 0.23721197E+02  
 4  
 C4H10OL C 4H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.94319448E+01 0.28290663E-01-0.97171314E-05 0.15629870E-08-0.96942494E-  
 13 2  
 -0.38785121E+05-0.21802601E+02 0.70391624E-03 0.51434118E-01-0.25048006E-  
 04 3  
 0.21933105E-09 0.28653735E-11-0.36071867E+05 0.27575392E+02  
 4  
 M102C5H12 C 5H 120 0 G 0300.00 5000.00 1000.00  
 1  
 0.68988895E+01 0.38945273E-01-0.14318298E-04 0.24153177E-08-0.15480237E-  
 12 2  
 -0.22808654E+05-0.10251524E+02-0.37944520E+00 0.54735661E-01-0.15632966E-  
 04 3  
 -0.12797436E-07 0.78605664E-11-0.20787176E+05 0.27959454E+02  
 4  
 C6H14 C 6H 140 0 G 0300.00 5000.00 1000.00  
 1  
 0.97638464E+01 0.43217782E-01-0.15517728E-04 0.25733407E-08-0.16292076E-  
 12 2  
 -0.27236531E+05-0.26481850E+02-0.44697708E+00 0.66306598E-01-0.22811577E-  
 04 3  
 -0.10950117E-07 0.77763932E-11-0.24345830E+05 0.27133120E+02  
 4  
 C4H10O2P C 4H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.12549208E+02 0.27114559E-01-0.90450494E-05 0.14250466E-08-0.87125016E-  
 13 2  
 -0.31024008E+05-0.32928814E+02 0.19046396E+01 0.52519988E-01-0.22357253E-  
 04 3  
 -0.57436043E-08 0.56328687E-11-0.27996590E+05 0.22811483E+02  
 4  
 C4H8O3AP C 4H 80 3 G 0300.00 5000.00 1000.00  
 1  
 0.14706219E+02 0.22925768E-01-0.76465558E-05 0.12043982E-08-0.73610897E-  
 13 2  
 -0.43085551E+05-0.41318802E+02 0.10041258E+01 0.63182734E-01-0.47795987E-  
 04 3  
 0.15303053E-07-0.57770656E-12-0.39552645E+05 0.28576126E+02  
 4  
 C3H6O3AP C 3H 60 3 G 0300.00 5000.00 1000.00  
 1  
 0.12695114E+02 0.16990611E-01-0.56055437E-05 0.87694280E-09-0.53389479E-  
 13 2  
 -0.39579113E+05-0.32484295E+02 0.12564497E+01 0.51121548E-01-0.40486342E-  
 04 3  
 0.13825359E-07-0.81327897E-12-0.36664109E+05 0.25714497E+02  
 4

C4H8O4PB                    C    4H    8O    4            G   0300.00    5000.00    1000.00  
1  
0.16783054E+02 0.23320194E-01-0.76735796E-05 0.11956303E-08-0.72449777E-  
13        2  
-0.74552797E+05-0.52034580E+02 0.23361542E+01 0.58531158E-01-0.21750257E-  
04        3  
-0.18100836E-07 0.12536630E-10-0.70716852E+05 0.22868334E+02  
4  
C3H6O4PB                    C    3H    6O    4            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C4H6Z2                      C    4H    6O    0            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C4H8Z                        C    4H    8O    0            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C4H8Y                        C    4H    8O    0            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C6H12Z                      C    6H    12O    0            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C7H14Z                      C    7H    14O    0            G   0300.00    5000.00    1000.00  
1  
0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
13        2  
-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
04        3  
-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
4  
C8H16Z                      C    8H    16O    0            G   0300.00    5000.00    1000.00  
1

0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C6H12OA C 6H 12O 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C7H14OA C 7H 14O 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C5H8Z2 C 5H 8O 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C3H4Z2 C 3H 4O 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C3H6OLY C 3H 6O 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C3H6O2PY C 3H 6O 2 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C4H6OAY C 4H 6O 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2

-0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C4H8OLY C 4H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C6H10Y2 C 6H 100 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C7H12Y2 C 7H 120 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C8H14Y2 C 8H 140 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C4H8O2PY C 4H 80 2 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C5H8OAY C 5H 80 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C5H10OLY C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3

-0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C9H16Y2 C 9H 160 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C5H10O2PY C 5H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C6H10OAY C 6H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C6H12OLY C 6H 120 1 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C10H18Y2 C 10H 180 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C3H6Z C 3H 60 0 G 0300.00 5000.00 1000.00  
 1  
 0.14778272E+02 0.17389165E-01-0.56439226E-05 0.87207763E-09-0.52605215E-  
 13 2  
 -0.71052461E+05-0.43243496E+02 0.23633287E+01 0.48020758E-01-0.18112594E-  
 04 3  
 -0.15994132E-07 0.11065627E-10-0.67804180E+05 0.20961147E+02  
 4  
 C2H4OE#3 C 2H 40 1 G 0300.00 5000.00 1000.00  
 1  
 0.43068867E+01 0.13877206E-01-0.51784232E-05 0.88229646E-09-0.56921298E-  
 13 2  
 -0.86772812E+04-0.38457742E+00-0.92033523E+00 0.26421962E-01-0.13407433E-  
 04 3  
 0.31399369E-09 0.14228568E-11-0.71333140E+04 0.27113031E+02  
 4

C3H6OE#3                    C    3H    6O    1            G   0300.00    5000.00    1000.00  
 1  
   0.70665474E+01  0.18753586E-01-0.67436472E-05  0.11200114E-08-0.71012281E-  
 13        2  
 -0.14982560E+05-0.13086255E+02  0.74423306E-01  0.35190679E-01-0.25911300E-  
 04        3  
   0.17298602E-07-0.65269183E-11-0.12573230E+05  0.24581474E+02  
 4  
 C3H6OE#4                    C    3H    6O    1            G   0300.00    5000.00    1000.00  
 1  
   0.40322506E+00  0.32915182E-01-0.14498929E-04  0.27762874E-08-0.19458094E-  
 12        2  
 -0.11845447E+05  0.19478727E+02  0.42862228E+00  0.19593410E-01  0.25290266E-  
 04        3  
 -0.38973763E-07  0.15062649E-10-0.11086957E+05  0.22832840E+02  
 4  
 C4H8OE#3                    C    4H    8O    1            G   0300.00    5000.00    1000.00  
 1  
   0.10053115E+02  0.23960005E-01-0.85541296E-05  0.14132795E-08-0.89266078E-  
 13        2  
 -0.18836031E+05-0.28119183E+02  0.35547379E+00  0.42264439E-01-0.80039545E-  
 05        3  
 -0.15980326E-07  0.81473717E-11-0.15772924E+05  0.24028938E+02  
 4  
 C4H8OE#4                    C    4H    8O    1            G   0300.00    5000.00    1000.00  
 1  
   0.33293636E+01  0.37815239E-01-0.16010379E-04  0.29808809E-08-0.20474120E-  
 12        2  
 -0.18223459E+05  0.56811781E+01-0.80936937E+01  0.88622943E-01-0.11073386E-  
 03        3  
   0.82279641E-07-0.24164665E-10-0.15662465E+05  0.60699963E+02  
 4  
 C4H8OE#5                    C    4H    8O    1            G   0300.00    5000.00    1000.00  
 1  
   0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  
 0.00000000E+00        2  
 -0.22193549E+05  0.18116014E+02  0.00000000E+00  0.00000000E+00  
 0.00000000E+00        3  
   0.00000000E+00  0.00000000E+00-0.22193549E+05  0.18116014E+02  
 4  
 M9C5H10OE#3                C    5H    10O    1            G   0300.00    5000.00    1000.00  
 1  
   0.12056057E+02  0.29910566E-01-0.10606705E-04  0.17437318E-08-0.10974145E-  
 12        2  
 -0.22338980E+05-0.36908218E+02  0.18163344E+00  0.53779867E-01-0.14001005E-  
 04        3  
 -0.15812684E-07  0.88460992E-11-0.18669836E+05  0.26558422E+02  
 4  
 M7C5H10OE#3                C    5H    10O    1            G   0300.00    5000.00    1000.00  
 1  
   0.12780155E+02  0.29217916E-01-0.10352643E-04  0.17017265E-08-0.10712660E-  
 12        2  
 -0.25083791E+05-0.42149376E+02-0.38458031E+00  0.58752142E-01-0.22541346E-  
 04        3  
 -0.10100603E-07  0.75144153E-11-0.21196994E+05  0.27378244E+02  
 4  
 M12C5H10OE#4                C    5H    10O    1            G   0300.00    5000.00    1000.00  
 1



0.55430174E+01 0.43825392E-01-0.18080451E-04 0.33056706E-08-0.22413904E-  
 12 2  
 -0.24252398E+05-0.68173380E+01-0.87576046E+01 0.10453284E+00-0.12373093E-  
 03 3  
 0.86439428E-07-0.24114238E-10-0.21094090E+05 0.62346928E+02  
 4  
 M8C5H10OE#4 C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.48403635E+01 0.44480752E-01-0.18311463E-04 0.33419503E-08-0.22626486E-  
 12 2  
 -0.21244830E+05-0.31016234E+00-0.82881823E+01 0.10023287E+00-0.11680756E-  
 03 3  
 0.82342609E-07-0.23354397E-10-0.18284848E+05 0.63323032E+02  
 4  
 M10C5H10OE#5 C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.75738430E+01 0.36838327E-01-0.13914652E-04 0.23919642E-08-0.15532837E-  
 12 2  
 -0.31961199E+05-0.16198759E+02-0.89854517E+01 0.93305685E-01-0.88499663E-  
 04 3  
 0.46996604E-07-0.10083021E-10-0.27939535E+05 0.66627655E+02  
 4  
 M11C5H10OE#6 C 5H 100 1 G 0300.00 5000.00 1000.00  
 1  
 0.61490073E+01 0.40091213E-01-0.15658075E-04 0.27557003E-08-0.18193188E-  
 12 2  
 -0.31798959E+05-0.11050709E+02-0.47018085E+01 0.61360236E-01-0.13543016E-  
 04 3  
 -0.22668338E-07 0.12708840E-10-0.28509820E+05 0.46829506E+02  
 4  
 M22C6H10O2E#3A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.16145472E+02 0.31791709E-01-0.11331013E-04 0.18699551E-08-0.11802436E-  
 12 2  
 -0.37872023E+05-0.54382687E+02-0.35935152E+00 0.72314717E-01-0.36872949E-  
 04 3  
 -0.29099245E-08 0.61856054E-11-0.33180484E+05 0.31893940E+02  
 4  
 M20C6H10O2E#3A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.16427986E+02 0.30794756E-01-0.10784026E-04 0.17574746E-08-0.10994830E-  
 12 2  
 -0.38603949E+05-0.55458248E+02 0.44225636E+00 0.72197743E-01-0.43107320E-  
 04 3  
 0.57066596E-08 0.28469037E-11-0.34123949E+05 0.27670315E+02  
 4  
 M17C6H10O2E#3A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.16418262E+02 0.30813152E-01-0.10794892E-04 0.17600429E-08-0.11015856E-  
 12 2  
 -0.38872152E+05-0.55404827E+02 0.43077764E+00 0.72277278E-01-0.43296957E-  
 04 3  
 0.58934342E-08 0.27818754E-11-0.34394465E+05 0.27718910E+02  
 4  
 M13C6H10O2E#3A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.15696230E+02 0.31493433E-01-0.11041287E-04 0.18002166E-08-0.11262461E-  
 12 2

-0.36397453E+05-0.50169853E+02 0.12212688E+01 0.65750793E-01-0.31028798E-  
 04 3  
 -0.35323338E-08 0.54250380E-11-0.32163062E+05 0.25949133E+02  
 4  
 M21C6H1002E#4A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.89035225E+01 0.46401165E-01-0.19057035E-04 0.34727470E-08-0.23489267E-  
 12 2  
 -0.36765559E+05-0.17634262E+02-0.86178474E+01 0.11730029E+00-0.13615201E-  
 03 3  
 0.91723493E-07-0.24768422E-10-0.32818078E+05 0.67763901E+02  
 4  
 M18C6H1002E#4A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.89050236E+01 0.45808949E-01-0.18649744E-04 0.33784051E-08-0.22758949E-  
 12 2  
 -0.37648488E+05-0.17109514E+02-0.77973824E+01 0.11702968E+00-0.14194494E-  
 03 3  
 0.99810634E-07-0.27882949E-10-0.34035035E+05 0.63463249E+02  
 4  
 M14C6H1002E#4A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.82145987E+01 0.46436563E-01-0.18865812E-04 0.34113978E-08-0.22945968E-  
 12 2  
 -0.34915469E+05-0.12052453E+02-0.71351805E+01 0.11139347E+00-0.13181665E-  
 03 3  
 0.92522598E-07-0.25996956E-10-0.31518170E+05 0.62236713E+02  
 4  
 M19C6H1002E#5A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.11674271E+02 0.38703684E-01-0.14635973E-04 0.25183955E-08-0.16367140E-  
 12 2  
 -0.47498539E+05-0.33735470E+02-0.94396362E+01 0.11124503E+00-0.10995781E-  
 03 3  
 0.58504892E-07-0.12255764E-10-0.42459562E+05 0.71594666E+02  
 4  
 M15C6H1002E#5A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.11195970E+02 0.38423836E-01-0.14323823E-04 0.24387357E-08-0.15725566E-  
 12 2  
 -0.45465613E+05-0.29347845E+02-0.79921432E+01 0.10558853E+00-0.10625012E-  
 03 3  
 0.59968848E-07-0.13737657E-10-0.40884199E+05 0.66215790E+02  
 4  
 M16C6H1002E#6A C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 0.10940360E+02 0.40857118E-01-0.15840807E-04 0.27711520E-08-0.18205318E-  
 12 2  
 -0.47648852E+05-0.31811312E+02-0.94919701E+01 0.10863237E+00-0.10302372E-  
 03 3  
 0.53701765E-07-0.11272679E-10-0.42557707E+05 0.70942215E+02  
 4  
 M32C6H1003E#3LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.18537668E+02 0.31721946E-01-0.11152513E-04 0.18228752E-08-0.11428857E-  
 12 2  
 -0.69495422E+05-0.66217346E+02-0.22544680E+01 0.89504771E-01-0.61495550E-  
 04 3

0.12008920E-07 0.30520137E-11-0.63993461E+05 0.40611416E+02  
 4  
 M30C6H1003E#3LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.18785324E+02 0.30794021E-01-0.10653136E-04 0.17225372E-08-0.10724311E-  
 12 2  
 -0.70214133E+05-0.67101608E+02-0.13407801E+01 0.88609554E-01-0.65859276E-  
 04 3  
 0.18758783E-07 0.37322226E-12-0.64948902E+05 0.35913265E+02  
 4  
 M27C6H1003E#3LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.18788137E+02 0.30784337E-01-0.10647106E-04 0.17210242E-08-0.10711204E-  
 12 2  
 -0.70485727E+05-0.67114418E+02-0.12419642E+01 0.87917916E-01-0.64182750E-  
 04 3  
 0.17070985E-07 0.97509370E-12-0.65231129E+05 0.35495663E+02  
 4  
 M23C6H1003E#3LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.18091894E+02 0.31426754E-01-0.10870080E-04 0.17554800E-08-0.10909919E-  
 12 2  
 -0.68023828E+05-0.62028168E+02-0.77183300E+00 0.83606862E-01-0.57219171E-  
 04 3  
 0.12922753E-07 0.17563400E-11-0.62965359E+05 0.35083500E+02  
 4  
 M31C6H1003E#4LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.11043774E+02 0.46697974E-01-0.19003113E-04 0.34411947E-08-0.23175420E-  
 12 2  
 -0.68282234E+05-0.28036964E+02-0.10692979E+02 0.13570362E+00-0.16358882E-  
 03 3  
 0.10933934E-06-0.28813091E-10-0.63611344E+05 0.77248360E+02  
 4  
 M28C6H1003E#4LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.11161845E+02 0.45890640E-01-0.18477673E-04 0.33203136E-08-0.22234683E-  
 12 2  
 -0.69207742E+05-0.28154156E+02-0.96445150E+01 0.13384928E+00-0.16557472E-  
 03 3  
 0.11362729E-06-0.30584552E-10-0.64852656E+05 0.71982536E+02  
 4  
 M24C6H1003E#4LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.10346826E+02 0.46757314E-01-0.18834764E-04 0.33867606E-08-0.22697058E-  
 12 2  
 -0.66430180E+05-0.22414549E+02-0.91979351E+01 0.12971301E+00-0.15905677E-  
 03 3  
 0.10994615E-06-0.29975293E-10-0.62312789E+05 0.71668465E+02  
 4  
 M29C6H1003E#5LK C 6H 100 3 G 0300.00 5000.00 1000.00  
 1  
 0.14060001E+02 0.38609307E-01-0.14412929E-04 0.24566016E-08-0.15854555E-  
 12 2  
 -0.79114625E+05-0.45518528E+02-0.11337935E+02 0.12843570E+00-0.13452662E-  
 03 3  
 0.73314077E-07-0.15330785E-10-0.73271906E+05 0.80328560E+02  
 4

M25C6H1003E#5LK                   C    6H  100   3           G  0300.00   5000.00   1000.00  
1  
0.13531691E+02  0.38438566E-01-0.14172049E-04  0.23948552E-08-0.15365083E-  
12       2  
-0.77338016E+05-0.40863544E+02-0.10094918E+02  0.12420744E+00-0.13427404E-  
03       3  
0.78249819E-07-0.18048891E-10-0.71946539E+05  0.75814232E+02  
4  
M26C6H1003E#6LK                   C    6H  100   3           G  0300.00   5000.00   1000.00  
1  
0.12194106E+02  0.42532109E-01-0.16453989E-04  0.28761584E-08-0.18896207E-  
12       2  
-0.78747352E+05-0.37162224E+02-0.41024303E+01  0.76532684E-01-0.13333481E-  
04       3  
-0.40376591E-07  0.22239240E-10-0.74163727E+05  0.48659966E+02  
4  
C4H6O2E#3A                         C    4H    60   2           G  0300.00   5000.00   1000.00  
1  
0.12205802E+02  0.19775139E-01-0.71629670E-05  0.11948924E-08-0.75945381E-  
13       2  
-0.31163959E+05-0.37173416E+02-0.47165025E-01  0.49530163E-01-0.25471598E-  
04       3  
-0.26518701E-08  0.45773910E-11-0.27654604E+05  0.26985292E+02  
4  
C4H6O2E#4A                         C    4H    60   2           G  0300.00   5000.00   1000.00  
1  
0.54490299E+01  0.33290446E-01-0.14483737E-04  0.27490950E-08-0.19145349E-  
12       2  
-0.27826047E+05-0.20500045E+01-0.79580922E+01  0.91174617E-01-0.12048168E-  
03       3  
0.90958608E-07-0.26880073E-10-0.24743016E+05  0.62946899E+02  
4  
C3H4O2E#3A                         C    3H    40   2           G  0300.00   5000.00   1000.00  
1  
0.94448385E+01  0.14590023E-01-0.54177990E-05  0.92055075E-09-0.59310006E-  
13       2  
-0.24904262E+05-0.22959730E+02  0.77175450E+00  0.32498680E-01-0.96391668E-  
05       3  
-0.98100728E-08  0.56571080E-11-0.22239012E+05  0.23301609E+02  
4  
C4H6O3E#3LK                        C    4H    60   3           G  0300.00   5000.00   1000.00  
1  
0.14561532E+02  0.19767018E-01-0.70146193E-05  0.11541548E-08-0.72699171E-  
13       2  
-0.62773039E+05-0.48804451E+02-0.19919444E+01  0.67053773E-01-0.50868803E-  
04       3  
0.13015145E-07  0.11872151E-11-0.58462109E+05  0.35914612E+02  
4  
C4H6O3E#4LK                        C    4H    60   3           G  0300.00   5000.00   1000.00  
1  
0.58960752E+01  0.36240067E-01-0.15690503E-04  0.29679486E-08-0.20618736E-  
12       2  
-0.58568656E+05-0.28337593E+01  0.10644912E+01  0.34465469E-01  0.26364327E-  
04       3  
-0.57714654E-07  0.25027768E-10-0.56744191E+05  0.25207870E+02  
4  
C3H4O3E#3LK                        C    3H    40   3           G  0300.00   5000.00   1000.00  
1

0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C6H12OE#3 C 6H 120 1 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C7H14OE#3 C 7H 140 1 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C8H16OE#3 C 8H 160 1 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C5H8O4E#4KP C 5H 80 4 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C5H8O4E#5KP C 5H 80 4 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 C5H8O4E#6KP C 5H 80 4 G 0300.00 5000.00 1000.00  
 1  
 0.11788570E+02 0.14572146E-01-0.52410855E-05 0.86980723E-09-0.55078463E-  
 13 2  
 -0.56501547E+05-0.34508099E+02-0.69039148E+00 0.46766605E-01-0.27510128E-  
 04 3  
 -0.12961724E-08 0.46644468E-11-0.53099207E+05 0.30175692E+02  
 4  
 R26C5H11 C 5H 110 0 G 0300.00 5000.00 1000.00  
 1  
 0.80374537E+01 0.32405894E-01-0.10609607E-04 0.16498065E-08-0.99973828E-  
 13 2

0.17401665E+04-0.12860074E+02-0.99321896E+00 0.64496689E-01-0.50283154E-  
 04 3  
 0.21544087E-07-0.33808297E-11 0.36325586E+04 0.31456369E+02  
 4  
 R27C5H11 C 5H 110 0 G 0300.00 5000.00 1000.00  
 1  
 0.87105532E+01 0.31877510E-01-0.10431868E-04 0.16204416E-08-0.98059575E-  
 13 2  
 0.25420979E+04-0.16085539E+02-0.45957428E+00 0.60749386E-01-0.40063725E-  
 04 3  
 0.11617876E-07-0.16538332E-12 0.46676797E+04 0.29887865E+02  
 4  
 R28C5H11 C 5H 110 0 G 0300.00 5000.00 1000.00  
 1  
 0.81053381E+01 0.32415539E-01-0.10625447E-04 0.16533985E-08-0.10022477E-  
 12 2  
 0.16534244E+04-0.12558491E+02 0.14618000E+00 0.57361599E-01-0.35735091E-  
 04 3  
 0.94185655E-08 0.25734991E-12 0.34966270E+04 0.27352406E+02  
 4  
 R29C6H11OK C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.16622210E+02 0.26402740E-01-0.77751956E-05 0.11219550E-08-0.64630938E-  
 13 2  
 -0.19739314E+05-0.54072285E+02 0.22432382E+01 0.59083089E-01-0.29667130E-  
 04 3  
 0.27081930E-08 0.19396869E-11-0.15200631E+05 0.22489923E+02  
 4  
 R30C6H11OA C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.17465611E+02 0.25429556E-01-0.73849815E-05 0.10522682E-08-0.59948093E-  
 13 2  
 -0.13359747E+05-0.58314320E+02-0.62549269E+00 0.80460675E-01-0.75145450E-  
 04 3  
 0.41910443E-07-0.10097670E-10-0.84043799E+04 0.34393749E+02  
 4  
 R31C6H11OA C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.16856064E+02 0.25967833E-01-0.75776479E-05 0.10850322E-08-0.62106353E-  
 13 2  
 -0.14244721E+05-0.54758663E+02 0.12984879E+00 0.76019682E-01-0.68251335E-  
 04 3  
 0.37119602E-07-0.87486242E-11-0.95912070E+04 0.31227039E+02  
 4  
 R32C6H11OA C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.17061600E+02 0.25560405E-01-0.74011582E-05 0.10542540E-08-0.60151232E-  
 13 2  
 -0.14276495E+05-0.55792572E+02-0.10124401E+01 0.84109209E-01-0.86551547E-  
 04 3  
 0.54070352E-07-0.14400626E-10-0.94793242E+04 0.35997948E+02  
 4  
 R33C6H11OA C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.17077805E+02 0.25528619E-01-0.73822848E-05 0.10497405E-08-0.59776552E-  
 13 2  
 -0.14282113E+05-0.55880909E+02-0.98241782E+00 0.83892576E-01-0.86011445E-  
 04 3

0.53513340E-07-0.14197950E-10-0.94824141E+04 0.35871990E+02  
 4  
 R34C6H110A C 6H 110 1 G 0300.00 5000.00 1000.00  
 1  
 0.16995117E+02 0.26630299E-01-0.79600341E-05 0.11613147E-08-0.67422156E-  
 13 2  
 -0.17572348E+05-0.58002800E+02-0.57919127E+00 0.79781950E-01-0.73149931E-  
 04 3  
 0.40478088E-07-0.97716401E-11-0.12732248E+05 0.32159985E+02  
 4  
 R35C6H1102K C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18483034E+02 0.26978523E-01-0.78861258E-05 0.11290044E-08-0.64529918E-  
 13 2  
 -0.41909414E+05-0.64861824E+02-0.20285847E+01 0.86697541E-01-0.72805626E-  
 04 3  
 0.31978612E-07-0.52020363E-11-0.36302371E+05 0.40569324E+02  
 4  
 R36C6H1102B C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.19665455E+02 0.25724839E-01-0.74225122E-05 0.10535097E-08-0.59900327E-  
 13 2  
 -0.44912531E+05-0.69087990E+02-0.25754731E+01 0.98015323E-01-0.10060266E-  
 03 3  
 0.57620536E-07-0.13496336E-10-0.39211270E+05 0.43349922E+02  
 4  
 R37C6H1102B C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.19055254E+02 0.26269097E-01-0.76197712E-05 0.10876169E-08-0.62187790E-  
 13 2  
 -0.45798465E+05-0.65531509E+02-0.19070019E+01 0.94185084E-01-0.95193747E-  
 04 3  
 0.54327547E-07-0.12681873E-10-0.40388922E+05 0.40549908E+02  
 4  
 R38C6H1102B C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.19292170E+02 0.25799084E-01-0.74063892E-05 0.10479897E-08-0.59494259E-  
 13 2  
 -0.45840758E+05-0.66735802E+02-0.29371083E+01 0.10148879E+00-0.11158919E-  
 03 3  
 0.69362429E-07-0.17651564E-10-0.40288930E+05 0.44846844E+02  
 4  
 R39C6H1102B C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.19236332E+02 0.25901603E-01-0.74667064E-05 0.10622671E-08-0.60667718E-  
 13 2  
 -0.45819469E+05-0.66427032E+02-0.29204531E+01 0.10136776E+00-0.11128547E-  
 03 3  
 0.69047140E-07-0.17536157E-10-0.40290633E+05 0.44777088E+02  
 4  
 R40C6H1102B C 6H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.19229408E+02 0.26865760E-01-0.79636047E-05 0.11549194E-08-0.66777794E-  
 13 2  
 -0.48128844E+05-0.69160278E+02-0.24521060E+01 0.96978195E-01-0.97928627E-  
 04 3  
 0.55608695E-07-0.12986451E-10-0.42544719E+05 0.40559055E+02  
 4

R41C3H7O2U C 3H 70 2 G 0300.00 5000.00 1000.00  
1  
0.13503214E+02 0.13771964E-01-0.35621306E-05 0.46638027E-09-0.25058699E-  
13 2  
-0.10972646E+05-0.42340824E+02 0.34593359E+00 0.47804203E-01-0.34433560E-  
04 3  
0.11472139E-07-0.10343456E-11-0.70905918E+04 0.26533663E+02  
4  
R42C4H9O2U C 4H 90 2 G 0300.00 5000.00 1000.00  
1  
0.15602375E+02 0.19481253E-01-0.54285274E-05 0.75312029E-09-0.42252778E-  
13 2  
-0.14502155E+05-0.51627148E+02 0.24988347E+00 0.58799535E-01-0.39250695E-  
04 3  
0.10553014E-07 0.14231263E-13-0.99960186E+04 0.28736156E+02  
4  
R43C5H11O2U C 5H 110 2 G 0300.00 5000.00 1000.00  
1  
0.17902100E+02 0.25252532E-01-0.73544652E-05 0.10514271E-08-0.60109863E-  
13 2  
-0.20246381E+05-0.63142120E+02 0.45702310E+01 0.41049715E-01 0.25613848E-  
04 3  
-0.59279056E-07 0.24836746E-10-0.15699293E+05 0.10555774E+02  
4  
R44C5H11O2U C 5H 110 2 G 0300.00 5000.00 1000.00  
1  
0.17699362E+02 0.25206689E-01-0.73175647E-05 0.10446389E-08-0.59711967E-  
13 2  
-0.18031562E+05-0.60906883E+02 0.37462369E+00 0.68274647E-01-0.40443552E-  
04 3  
0.60420766E-08 0.23256178E-11-0.12925232E+05 0.30001059E+02  
4  
R45C5H11O2U C 5H 110 2 G 0300.00 5000.00 1000.00  
1  
0.17902794E+02 0.25252532E-01-0.73544652E-05 0.10514271E-08-0.60109863E-  
13 2  
-0.20518750E+05-0.62452854E+02 0.45328522E+01 0.41307453E-01 0.24998693E-  
04 3  
-0.58668839E-07 0.24622018E-10-0.15967014E+05 0.11408155E+02  
4  
R46C6H11O3AU C 6H 110 3 G 0300.00 5000.00 1000.00  
1  
0.21335835E+02 0.26828464E-01-0.77923196E-05 0.11119620E-08-0.63496178E-  
13 2  
-0.31825111E+05-0.74160202E+02 0.80790561E+00 0.84354684E-01-0.67032299E-  
04 3  
0.27487630E-07-0.41974753E-11-0.26080754E+05 0.31977087E+02  
4  
R47C4H7OA C 4H 70 1 G 0300.00 5000.00 1000.00  
1  
0.13303379E+02 0.13959693E-01-0.36331946E-05 0.47900761E-09-0.25924458E-  
13 2  
-0.63155015E+04-0.39949265E+02-0.44478342E+00 0.58604494E-01-0.66025204E-  
04 3  
0.44507157E-07-0.12558702E-10-0.25928850E+04 0.30028027E+02  
4  
R48C6H11O3AU C 6H 110 3 G 0300.00 5000.00 1000.00  
1



0.22038982E+02 0.26181309E-01-0.75696012E-05 0.10771060E-08-0.61410539E-  
 13 2  
 -0.34562906E+05-0.78593300E+02 0.26549503E+00 0.89165293E-01-0.75193675E-  
 04 3  
 0.32831792E-07-0.54025209E-11-0.28610504E+05 0.33391056E+02  
 4  
 R49C3H50A C 3H 50 1 G 0300.00 5000.00 1000.00  
 1  
 0.11188816E+02 0.83578881E-02-0.18887911E-05 0.22385428E-09-0.11240713E-  
 13 2  
 -0.27902478E+04-0.30617746E+02-0.27334598E+00 0.47125604E-01-0.60177084E-  
 04 3  
 0.44561723E-07-0.13366371E-10 0.30404608E+03 0.27495989E+02  
 4  
 R50C6H1103AU C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22038166E+02 0.26181309E-01-0.75696012E-05 0.10771060E-08-0.61410539E-  
 13 2  
 -0.34290418E+05-0.78589005E+02 0.29782385E+00 0.88935822E-01-0.74630188E-  
 04 3  
 0.32258313E-07-0.51962020E-11-0.28342146E+05 0.33253700E+02  
 4  
 R51C6H1103AU C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22010809E+02 0.26230784E-01-0.75989014E-05 0.10840780E-08-0.61985810E-  
 13 2  
 -0.34279770E+05-0.78437553E+02 0.34121788E+00 0.88639058E-01-0.73926509E-  
 04 3  
 0.31563228E-07-0.49522127E-11-0.28346857E+05 0.33069054E+02  
 4  
 R52C6H1103AU C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.21980928E+02 0.26735006E-01-0.78369303E-05 0.11247233E-08-0.64419742E-  
 13 2  
 -0.25487789E+05-0.78745415E+02-0.59784353E+00 0.89716166E-01-0.70017086E-  
 04 3  
 0.25287203E-07-0.24491331E-11-0.19236557E+05 0.37874153E+02  
 4  
 R53C6H1104UB C 6H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.23605429E+02 0.27017657E-01-0.77827954E-05 0.11044355E-08-0.62848449E-  
 13 2  
 -0.63407980E+05-0.85331703E+02-0.12860715E+01 0.10291510E+00-0.94924391E-  
 04 3  
 0.45648225E-07-0.84709861E-11-0.56872324E+05 0.41540150E+02  
 4  
 R54C4H702B C 4H 70 2 G 0300.00 5000.00 1000.00  
 1  
 0.15427574E+02 0.14378823E-01-0.37300399E-05 0.49159854E-09-0.26652317E-  
 13 2  
 -0.37837621E+05-0.50294891E+02-0.23624182E+01 0.75924061E-01-0.90886548E-  
 04 3  
 0.59587020E-07-0.15720812E-10-0.33403102E+05 0.38852104E+02  
 4  
 R55C6H1104UB C 6H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.24327904E+02 0.26333623E-01-0.75390572E-05 0.10646557E-08-0.60358680E-  
 13 2

-0.66152617E+05-0.89870552E+02-0.17676133E+01 0.10731147E+00-0.10210845E-  
 03 3  
 0.50032547E-07-0.93411927E-11-0.59408703E+05 0.42695320E+02  
 4  
 R56C3H5O2B C 3H 50 2 G 0300.00 5000.00 1000.00  
 1  
 0.13256764E+02 0.88558299E-02-0.20110283E-05 0.23953006E-09-0.12087953E-  
 13 2  
 -0.34287797E+05-0.40638344E+02-0.21509118E+01 0.64166412E-01-0.84363666E-  
 04 3  
 0.58959127E-07-0.16281953E-10-0.30510459E+05 0.36154118E+02  
 4  
 R57C6H11O4UB C 6H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.24327450E+02 0.26333623E-01-0.75390572E-05 0.10646557E-08-0.60358680E-  
 13 2  
 -0.65880469E+05-0.89868805E+02-0.17454053E+01 0.10715678E+00-0.10173616E-  
 03 3  
 0.49660734E-07-0.92096417E-11-0.59139328E+05 0.42600117E+02  
 4  
 R58C6H11O4UB C 6H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.24369911E+02 0.26259601E-01-0.74961104E-05 0.10546005E-08-0.59539430E-  
 13 2  
 -0.65897680E+05-0.90106316E+02-0.18491628E+01 0.10787600E+00-0.10346370E-  
 03 3  
 0.51385648E-07-0.98203286E-11-0.59128215E+05 0.43039204E+02  
 4  
 R59C6H11O4UB C 6H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.23825434E+02 0.27532309E-01-0.80738691E-05 0.11606276E-08-0.66635662E-  
 13 2  
 -0.65015176E+05-0.87471832E+02 0.88408011E+00 0.84070258E-01-0.41736712E-  
 04 3  
 -0.10151932E-07 0.11312172E-10-0.58569469E+05 0.32221054E+02  
 4  
 R60C3H7O2P C 3H 70 2 G 0300.00 5000.00 1000.00  
 1  
 0.13672139E+02 0.12750814E-01-0.31189277E-05 0.39289025E-09-0.20614268E-  
 13 2  
 -0.49886187E+04-0.39165993E+02 0.15149921E+01 0.48824649E-01-0.45656896E-  
 04 3  
 0.24564915E-07-0.55713593E-11-0.16219240E+04 0.23338097E+02  
 4  
 R61C3H7O2P C 3H 70 2 G 0300.00 5000.00 1000.00  
 1  
 0.14200809E+02 0.12368476E-01-0.30191270E-05 0.38157991E-09-0.20166079E-  
 13 2  
 -0.40745940E+04-0.42278625E+02 0.64384925E+00 0.54055225E-01-0.54415486E-  
 04 3  
 0.31187664E-07-0.75596803E-11-0.42250775E+03 0.26997149E+02  
 4  
 R62C4H9O2P C 4H 90 2 G 0300.00 5000.00 1000.00  
 1  
 0.16071844E+02 0.17864266E-01-0.46945179E-05 0.62312139E-09-0.33868511E-  
 13 2  
 -0.85830020E+04-0.50002316E+02 0.41746065E+00 0.66929147E-01-0.66410845E-  
 04 3

0.38230098E-07-0.93350154E-11-0.44304644E+04 0.29717245E+02  
 4  
 R63C4H9O2P C 4H 90 2 G 0300.00 5000.00 1000.00  
 1  
 0.15863925E+02 0.18276053E-01-0.48705583E-05 0.65426875E-09-0.35914597E-  
 13 2  
 -0.85510176E+04-0.48955978E+02 0.14225247E+01 0.59792988E-01-0.50404382E-  
 04 3  
 0.23572246E-07-0.44956040E-11-0.45277007E+04 0.25527254E+02  
 4  
 R64C4H9O2P C 4H 90 2 G 0300.00 5000.00 1000.00  
 1  
 0.16415470E+02 0.17848140E-01-0.47433541E-05 0.63675132E-09-0.34983135E-  
 13 2  
 -0.76448638E+04-0.52193089E+02 0.60832828E+00 0.64633384E-01-0.58237252E-  
 04 3  
 0.29281617E-07-0.61640532E-11-0.33344470E+04 0.28944464E+02  
 4  
 R65C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18210478E+02 0.23947487E-01-0.67307633E-05 0.93793984E-09-0.52691758E-  
 13 2  
 -0.14310736E+05-0.60030693E+02 0.57950335E+01 0.41689478E-01 0.15292435E-  
 04 3  
 -0.47076437E-07 0.20611939E-10-0.10236686E+05 0.78172021E+01  
 4  
 R66C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18771378E+02 0.23497580E-01-0.65901481E-05 0.91738317E-09-0.51525516E-  
 13 2  
 -0.13406875E+05-0.63316662E+02 0.50832539E+01 0.45818452E-01 0.91703050E-  
 05 3  
 -0.43075772E-07 0.19548429E-10-0.90543730E+04 0.10800845E+02  
 4  
 R67C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18219748E+02 0.23485268E-01-0.65141744E-05 0.89930724E-09-0.50209694E-  
 13 2  
 -0.12130488E+05-0.59557983E+02 0.46351600E+00 0.76954529E-01-0.68934860E-  
 04 3  
 0.35055390E-07-0.74986363E-11-0.73513271E+04 0.31315548E+02  
 4  
 R68C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18211142E+02 0.23501348E-01-0.65232957E-05 0.90142627E-09-0.50382370E-  
 13 2  
 -0.12127276E+05-0.59510456E+02 0.41875389E+00 0.77245265E-01-0.69588270E-  
 04 3  
 0.35668727E-07-0.77042374E-11-0.73462437E+04 0.31507940E+02  
 4  
 R69C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18011354E+02 0.23902215E-01-0.66944849E-05 0.93115105E-09-0.52278270E-  
 13 2  
 -0.12099247E+05-0.58511318E+02 0.14070796E+01 0.70242055E-01-0.53939111E-  
 04 3  
 0.21400107E-07-0.30121725E-11-0.74419429E+04 0.27386412E+02  
 4

R70C5H1102P                    C    5H   110   2           G   0300.00    5000.00   1000.00  
1  
0.18570549E+02 0.23457348E-01-0.65568925E-05 0.91130709E-09-0.51169931E-  
13        2  
-0.11195259E+05-0.61788998E+02 0.64285290E+00 0.74731119E-01-0.60917569E-  
04        3  
0.26247735E-07-0.43729946E-11-0.62539648E+04 0.30592690E+02  
4  
R71C5H1102P                    C    5H   110   2           G   0300.00    5000.00   1000.00  
1  
0.18752226E+02 0.23536196E-01-0.66126163E-05 0.92265695E-09-0.51956120E-  
13        2  
-0.14024604E+05-0.63212952E+02 0.49879084E+01 0.46478335E-01 0.75884550E-  
05        3  
-0.41499785E-07 0.18991593E-10-0.96681465E+04 0.11204841E+02  
4  
R72C5H1102P                    C    5H   110   2           G   0300.00    5000.00   1000.00  
1  
0.18420027E+02 0.23533041E-01-0.65516374E-05 0.90639368E-09-0.50651208E-  
13        2  
-0.14615505E+05-0.61086559E+02 0.46930351E+01 0.49489446E-01-0.22892000E-  
05        3  
-0.30863038E-07 0.15226929E-10-0.10400687E+05 0.12418933E+02  
4  
R73C5H1102P                    C    5H   110   2           G   0300.00    5000.00   1000.00  
1  
0.18210478E+02 0.23947487E-01-0.67307633E-05 0.93793984E-09-0.52691758E-  
13        2  
-0.14582478E+05-0.60030689E+02 0.57950335E+01 0.41689478E-01 0.15292435E-  
04        3  
-0.47076437E-07 0.20611939E-10-0.10508427E+05 0.78172059E+01  
4  
R74C5H1102P                    C    5H   110   2           G   0300.00    5000.00   1000.00  
1  
0.18771378E+02 0.23497580E-01-0.65901481E-05 0.91738317E-09-0.51525516E-  
13        2  
-0.13678615E+05-0.63316658E+02 0.50832539E+01 0.45818452E-01 0.91703050E-  
05        3  
-0.43075772E-07 0.19548429E-10-0.93261143E+04 0.10800849E+02  
4  
R75C6H1103AP                    C    6H   110   3           G   0300.00    5000.00   1000.00  
1  
0.21817451E+02 0.25182672E-01-0.70321253E-05 0.97680952E-09-0.54833779E-  
13        2  
-0.25910752E+05-0.72599327E+02 0.75295585E+00 0.94032779E-01-0.97924167E-  
04        3  
0.58901389E-07-0.14872983E-10-0.20491477E+05 0.33901310E+02  
4  
R76C6H1103AP                    C    6H   110   3           G   0300.00    5000.00   1000.00  
1  
0.21817451E+02 0.25182672E-01-0.70321253E-05 0.97680952E-09-0.54833779E-  
13        2  
-0.25910752E+05-0.72599327E+02 0.75295585E+00 0.94032779E-01-0.97924167E-  
04        3  
0.58901389E-07-0.14872983E-10-0.20491477E+05 0.33901310E+02  
4  
R77C6H1103AP                    C    6H   110   3           G   0300.00    5000.00   1000.00  
1

0.21783941E+02 0.25240153E-01-0.70669394E-05 0.98524211E-09-0.55539418E-  
 13 2  
 -0.25896660E+05-0.72411308E+02 0.89558333E+00 0.93036726E-01-0.95514828E-  
 04 3  
 0.56480228E-07-0.14010852E-10-0.20506643E+05 0.33298233E+02  
 4  
 R78C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.21766270E+02 0.26216384E-01-0.75661087E-05 0.10787923E-08-0.61785456E-  
 13 2  
 -0.29210457E+05-0.74858475E+02 0.12277572E+01 0.89443281E-01-0.83910949E-  
 04 3  
 0.44699583E-07-0.10026120E-10-0.23749443E+05 0.29912888E+02  
 4  
 R79C4H703AU C 4H 70 3 G 0300.00 5000.00 1000.00  
 1  
 0.17023647E+02 0.15579970E-01-0.41271032E-05 0.55305738E-09-0.30366788E-  
 13 2  
 -0.24716369E+05-0.54935658E+02 0.11403732E+01 0.61437923E-01-0.55336895E-  
 04 3  
 0.27478016E-07-0.57202142E-11-0.20285412E+05 0.26976534E+02  
 4  
 R80C4H70K C 4H 70 1 G 0300.00 5000.00 1000.00  
 1  
 0.12437756E+02 0.14725862E-01-0.38871476E-05 0.51765459E-09-0.28199833E-  
 13 2  
 -0.12891049E+05-0.35555153E+02 0.97469956E+00 0.46792146E-01-0.41991694E-  
 04 3  
 0.24506681E-07-0.65159080E-11-0.94593340E+04 0.24240408E+02  
 4  
 R81C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22841780E+02 0.24559533E-01-0.68851400E-05 0.96189590E-09-0.54359203E-  
 13 2  
 -0.28053217E+05-0.79100128E+02 0.57643950E+00 0.95343046E-01-0.95037656E-  
 04 3  
 0.52441997E-07-0.11900117E-10-0.22296334E+05 0.33797546E+02  
 4  
 R82C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22475647E+02 0.24617311E-01-0.68595396E-05 0.95387664E-09-0.53722262E-  
 13 2  
 -0.28630838E+05-0.76785271E+02 0.30760550E+00 0.98162197E-01-0.10442856E-  
 03 3  
 0.62570592E-07-0.15478263E-10-0.23031504E+05 0.34902992E+02  
 4  
 R83C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22532766E+02 0.24516648E-01-0.68005875E-05 0.93996055E-09-0.52580519E-  
 13 2  
 -0.28653811E+05-0.77103683E+02 0.17167749E+00 0.99102765E-01-0.10668134E-  
 03 3  
 0.64811736E-07-0.16268631E-10-0.23016930E+05 0.35478931E+02  
 4  
 R84C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22582428E+02 0.25365101E-01-0.72240118E-05 0.10156949E-08-0.57375979E-  
 13 2

-0.31992199E+05-0.79913872E+02 0.56749189E+00 0.95072009E-01-0.94037408E-  
 04 3  
 0.52003653E-07-0.11923910E-10-0.26266600E+05 0.31830357E+02  
 4  
 R85C6H1103KP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22026375E+02 0.25241811E-01-0.70905498E-05 0.98854480E-09-0.55598009E-  
 13 2  
 -0.34297820E+05-0.74988586E+02 0.17867521E+01 0.84973082E-01-0.74448879E-  
 04 3  
 0.35861028E-07-0.70614009E-11-0.28788018E+05 0.28896959E+02  
 4  
 R86C3H503AU C 3H 50 3 G 0300.00 5000.00 1000.00  
 1  
 0.14811378E+02 0.10091698E-01-0.23944904E-05 0.29484665E-09-0.15227479E-  
 13 2  
 -0.21145572E+05-0.45028854E+02 0.13057311E+01 0.49984276E-01-0.49496310E-  
 04 3  
 0.27475785E-07-0.64812782E-11-0.17387633E+05 0.24479385E+02  
 4  
 R87C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22347456E+02 0.24882207E-01-0.69506427E-05 0.96463038E-09-0.54057931E-  
 13 2  
 -0.28357064E+05-0.76179245E+02 0.13853881E+01 0.90537786E-01-0.87287073E-  
 04 3  
 0.46813483E-07-0.10259992E-10-0.22865004E+05 0.30402758E+02  
 4  
 R88C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22841780E+02 0.24559533E-01-0.68851400E-05 0.96189590E-09-0.54359203E-  
 13 2  
 -0.27429217E+05-0.79100128E+02 0.57643950E+00 0.95343046E-01-0.95037656E-  
 04 3  
 0.52441997E-07-0.11900117E-10-0.21672334E+05 0.33797546E+02  
 4  
 R89C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22532766E+02 0.24516648E-01-0.68005875E-05 0.93996055E-09-0.52580519E-  
 13 2  
 -0.28382070E+05-0.77103683E+02 0.17167749E+00 0.99102765E-01-0.10668134E-  
 03 3  
 0.64811736E-07-0.16268631E-10-0.22745189E+05 0.35478931E+02  
 4  
 R90C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22580627E+02 0.25365101E-01-0.72240118E-05 0.10156949E-08-0.57375979E-  
 13 2  
 -0.31718809E+05-0.79899902E+02 0.65703231E+00 0.94450340E-01-0.92543101E-  
 04 3  
 0.50511751E-07-0.11395986E-10-0.26004430E+05 0.31453205E+02  
 4  
 R91C6H1103KP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22026375E+02 0.25241811E-01-0.70905498E-05 0.98854480E-09-0.55598009E-  
 13 2  
 -0.34026078E+05-0.74988586E+02 0.17867521E+01 0.84973082E-01-0.74448879E-  
 04 3

0.35861028E-07-0.70614009E-11-0.28516275E+05 0.28896959E+02  
 4  
 R92C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22581066E+02 0.25365101E-01-0.72240118E-05 0.10156949E-08-0.57375979E-  
 13 2  
 -0.31719209E+05-0.79898277E+02 0.63482434E+00 0.94605029E-01-0.92915405E-  
 04 3  
 0.50883560E-07-0.11527535E-10-0.26002068E+05 0.31551680E+02  
 4  
 R93C6H1103KP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22026375E+02 0.25241811E-01-0.70905498E-05 0.98854480E-09-0.55598009E-  
 13 2  
 -0.34026078E+05-0.74988586E+02 0.17867521E+01 0.84973082E-01-0.74448879E-  
 04 3  
 0.35861028E-07-0.70614009E-11-0.28516275E+05 0.28896959E+02  
 4  
 R94C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22530975E+02 0.24516039E-01-0.67999831E-05 0.93977826E-09-0.52563297E-  
 13 2  
 -0.28380293E+05-0.77091408E+02 0.27423498E+00 0.98393902E-01-0.10498614E-  
 03 3  
 0.63128233E-07-0.15675987E-10-0.22756195E+05 0.35044292E+02  
 4  
 R95C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22347456E+02 0.24882207E-01-0.69506427E-05 0.96463038E-09-0.54057931E-  
 13 2  
 -0.28357064E+05-0.76179245E+02 0.13853881E+01 0.90537786E-01-0.87287073E-  
 04 3  
 0.46813483E-07-0.10259992E-10-0.22865004E+05 0.30402758E+02  
 4  
 R96C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22841780E+02 0.24559533E-01-0.68851400E-05 0.96189590E-09-0.54359203E-  
 13 2  
 -0.27429217E+05-0.79100128E+02 0.57643950E+00 0.95343046E-01-0.95037656E-  
 04 3  
 0.52441997E-07-0.11900117E-10-0.21672334E+05 0.33797546E+02  
 4  
 R97C6H1103KP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.21914146E+02 0.25889795E-01-0.74117493E-05 0.10492853E-08-0.59730439E-  
 13 2  
 -0.33705340E+05-0.74837090E+02 0.10141631E+01 0.84892087E-01-0.67750458E-  
 04 3  
 0.26795849E-07-0.35698942E-11-0.27928209E+05 0.32997299E+02  
 4  
 R98C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
 1  
 0.22503725E+02 0.25006529E-01-0.70270589E-05 0.97819719E-09-0.54864760E-  
 13 2  
 -0.27739627E+05-0.77409294E+02-0.54905844E+00 0.98670676E-01-0.99159559E-  
 04 3  
 0.54942692E-07-0.12498224E-10-0.21810537E+05 0.39358471E+02  
 4

R99C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
1  
0.22503725E+02 0.25006529E-01-0.70270589E-05 0.97819719E-09-0.54864760E-  
13 2  
-0.27739627E+05-0.77409294E+02-0.54905844E+00 0.98670676E-01-0.99159559E-  
04 3  
0.54942692E-07-0.12498224E-10-0.21810537E+05 0.39358471E+02  
4  
R100C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
1  
0.22270023E+02 0.25464889E-01-0.72325006E-05 0.10159571E-08-0.57412171E-  
13 2  
-0.27697125E+05-0.76219414E+02 0.58235526E+00 0.90657733E-01-0.81044884E-  
04 3  
0.38177703E-07-0.69119506E-11-0.21921279E+05 0.34633427E+02  
4  
R101C6H1103AP C 6H 110 3 G 0300.00 5000.00 1000.00  
1  
0.22784315E+02 0.25108360E-01-0.71466861E-05 0.10083905E-08-0.57315691E-  
13 2  
-0.26777791E+05-0.79252609E+02-0.31740010E+00 0.96098125E-01-0.90334739E-  
04 3  
0.45355442E-07-0.91043640E-11-0.20718961E+05 0.38412060E+02  
4  
R102C6H1104PB C 6H 110 4 G 0300.00 5000.00 1000.00  
1  
0.24090248E+02 0.25356961E-01-0.70155693E-05 0.96745301E-09-0.54010192E-  
13 2  
-0.57491898E+05-0.83782227E+02-0.10276229E+01 0.11041945E+00-0.12059385E-  
03 3  
0.71847786E-07-0.17300687E-10-0.51316594E+05 0.42137421E+02  
4  
R103C6H1104PB C 6H 110 4 G 0300.00 5000.00 1000.00  
1  
0.24090248E+02 0.25356961E-01-0.70155693E-05 0.96745301E-09-0.54010192E-  
13 2  
-0.57491898E+05-0.83782227E+02-0.10276229E+01 0.11041945E+00-0.12059385E-  
03 3  
0.71847786E-07-0.17300687E-10-0.51316594E+05 0.42137421E+02  
4  
R104C6H1104PB C 6H 110 4 G 0300.00 5000.00 1000.00  
1  
0.24050516E+02 0.25439188E-01-0.70646074E-05 0.97919972E-09-0.54985388E-  
13 2  
-0.57479316E+05-0.84261215E+02-0.12484928E+01 0.11194766E+00-0.12425469E-  
03 3  
0.75491272E-07-0.18586445E-10-0.51292910E+05 0.42380222E+02  
4  
R105C6H1104PB C 6H 110 4 G 0300.00 5000.00 1000.00  
1  
0.24049301E+02 0.26378483E-01-0.75416988E-05 0.10676866E-08-0.60831690E-  
13 2  
-0.59787480E+05-0.86994766E+02-0.60982037E+00 0.10638896E+00-0.10809546E-  
03 3  
0.59254944E-07-0.13045686E-10-0.53565520E+05 0.37461277E+02  
4  
R106C4H7O4UB C 4H 7O 4 G 0300.00 5000.00 1000.00  
1



0.19258875E+02 0.15822969E-01-0.41468552E-05 0.55124011E-09-0.30094576E-  
 13 2  
 -0.56283793E+05-0.65910828E+02-0.72430068E+00 0.78404568E-01-0.79391612E-  
 04 3  
 0.41798788E-07-0.86313092E-11-0.51101477E+05 0.35569962E+02  
 4  
 R107C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.25129574E+02 0.24718150E-01-0.68595104E-05 0.95041652E-09-0.53362612E-  
 13 2  
 -0.59643383E+05-0.91066284E+02-0.15226643E+01 0.11393695E+00-0.12300619E-  
 03 3  
 0.70676620E-07-0.16199445E-10-0.53087316E+05 0.42689854E+02  
 4  
 R108C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24802971E+02 0.24700351E-01-0.67907081E-05 0.93233032E-09-0.51906182E-  
 13 2  
 -0.60235039E+05-0.88967911E+02-0.16947391E+01 0.11608433E+00-0.13078036E-  
 03 3  
 0.79186798E-07-0.19202988E-10-0.53832836E+05 0.43385582E+02  
 4  
 R109C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24813438E+02 0.24677204E-01-0.67761875E-05 0.92872915E-09-0.51599770E-  
 13 2  
 -0.60238023E+05-0.88330490E+02-0.16044990E+01 0.11546572E+00-0.12931463E-  
 03 3  
 0.77745121E-07-0.18700120E-10-0.53842586E+05 0.43695538E+02  
 4  
 R110C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24835989E+02 0.25580367E-01-0.72321122E-05 0.10124546E-08-0.57077817E-  
 13 2  
 -0.62557434E+05-0.91174889E+02-0.11742358E+01 0.11136215E+00-0.11667018E-  
 03 3  
 0.65032445E-07-0.14410565E-10-0.56093047E+05 0.39683002E+02  
 4  
 R111C3H5O4UB C 3H 5O 4 G 0300.00 5000.00 1000.00  
 1  
 0.17012077E+02 0.10399957E-01-0.24472827E-05 0.29959890E-09-0.15419205E-  
 13 2  
 -0.52701293E+05-0.55814800E+02-0.72701859E+00 0.68122923E-01-0.76380558E-  
 04 3  
 0.44633016E-07-0.10399431E-10-0.48185809E+05 0.33784405E+02  
 4  
 R112C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24546618E+02 0.25198301E-01-0.70178007E-05 0.97518749E-09-0.54878441E-  
 13 2  
 -0.59911926E+05-0.86958992E+02-0.52155477E+00 0.10780521E+00-0.11208446E-  
 03 3  
 0.61896742E-07-0.13448507E-10-0.53676648E+05 0.39173454E+02  
 4  
 R113C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.25196121E+02 0.24592251E-01-0.67854567E-05 0.93287045E-09-0.51918576E-  
 13 2

-0.59043707E+05-0.90738914E+02-0.14480091E+01 0.11342218E+00-0.12177755E-  
 03 3  
 0.69457840E-07-0.15770593E-10-0.52471352E+05 0.43066353E+02  
 4  
 R114C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24813438E+02 0.24677204E-01-0.67761875E-05 0.92872915E-09-0.51599770E-  
 13 2  
 -0.59966289E+05-0.89023567E+02-0.16044990E+01 0.11546572E+00-0.12931463E-  
 03 3  
 0.77745121E-07-0.18700120E-10-0.53570852E+05 0.43002457E+02  
 4  
 R115C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24836931E+02 0.25580367E-01-0.72321122E-05 0.10124546E-08-0.57077817E-  
 13 2  
 -0.62286547E+05-0.91867188E+02-0.12265807E+01 0.11172154E+00-0.11752485E-  
 03 3  
 0.65877764E-07-0.14707312E-10-0.55815656E+05 0.39219162E+02  
 4  
 R116C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24835236E+02 0.25580367E-01-0.72321122E-05 0.10124546E-08-0.57077817E-  
 13 2  
 -0.62284988E+05-0.91839767E+02-0.11481580E+01 0.11117359E+00-0.11619843E-  
 03 3  
 0.64544423E-07-0.14232565E-10-0.55823996E+05 0.38903641E+02  
 4  
 R117C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24813438E+02 0.24677204E-01-0.67761875E-05 0.92872915E-09-0.51599770E-  
 13 2  
 -0.59966289E+05-0.88330490E+02-0.16044990E+01 0.11546572E+00-0.12931463E-  
 03 3  
 0.77745121E-07-0.18700120E-10-0.53570852E+05 0.43695538E+02  
 4  
 R118C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24546618E+02 0.25198301E-01-0.70178007E-05 0.97518749E-09-0.54878441E-  
 13 2  
 -0.59911926E+05-0.86958992E+02-0.52155477E+00 0.10780521E+00-0.11208446E-  
 03 3  
 0.61896742E-07-0.13448507E-10-0.53676648E+05 0.39173454E+02  
 4  
 R119C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.25196121E+02 0.24592251E-01-0.67854567E-05 0.93287045E-09-0.51918576E-  
 13 2  
 -0.59043707E+05-0.90738914E+02-0.14480091E+01 0.11342218E+00-0.12177755E-  
 03 3  
 0.69457840E-07-0.15770593E-10-0.52471352E+05 0.43066353E+02  
 4  
 R120C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24337086E+02 0.25824165E-01-0.72766034E-05 0.10171221E-08-0.57328708E-  
 13 2  
 -0.59110398E+05-0.86073212E+02 0.96409762E+00 0.92808820E-01-0.70362046E-  
 04 3

0.18988462E-07 0.14451073E-11-0.52994578E+05 0.33573685E+02  
 4  
 R121C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24353153E+02 0.25796667E-01-0.72603866E-05 0.10132597E-08-0.57008997E-  
 13 2  
 -0.59117148E+05-0.86163361E+02 0.90789771E+00 0.93203127E-01-0.71317605E-  
 04 3  
 0.19947731E-07 0.11045331E-11-0.52988645E+05 0.33811001E+02  
 4  
 R122C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24120058E+02 0.26246736E-01-0.74614472E-05 0.10500997E-08-0.59489191E-  
 13 2  
 -0.59072734E+05-0.84972305E+02 0.22563272E+01 0.83689019E-01-0.49608647E-  
 04 3  
 -0.39260134E-09 0.79518588E-11-0.53122672E+05 0.28166380E+02  
 4  
 R123C6H11O4PB C 6H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24692396E+02 0.25785010E-01-0.73140354E-05 0.10279926E-08-0.58200115E-  
 13 2  
 -0.58175902E+05-0.88327286E+02 0.13050411E+01 0.89490332E-01-0.59772668E-  
 04 3  
 0.76633668E-08 0.54470929E-11-0.51914898E+05 0.32162720E+02  
 4  
 R124C3H7O4UP C 3H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.18906818E+02 0.12912722E-01-0.31142890E-05 0.38873985E-09-0.20298040E-  
 13 2  
 -0.25333242E+05-0.63994617E+02 0.14959549E+01 0.63019961E-01-0.55043904E-  
 04 3  
 0.22621872E-07-0.30201917E-11-0.20624432E+05 0.25471867E+02  
 4  
 R125C3H7O4UP C 3H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.18177813E+02 0.13586381E-01-0.33381091E-05 0.42327411E-09-0.22383283E-  
 13 2  
 -0.22581078E+05-0.58714561E+02 0.22698126E+01 0.56646202E-01-0.43273030E-  
 04 3  
 0.13861366E-07-0.67737602E-12-0.18119873E+05 0.23766033E+02  
 4  
 R126C4H9O4UP C 4H 9O 4 G 0300.00 5000.00 1000.00  
 1  
 0.21160191E+02 0.18341102E-01-0.48231136E-05 0.64272282E-09-0.35146416E-  
 13 2  
 -0.28650328E+05-0.73444031E+02 0.12464113E+01 0.75056180E-01-0.62279512E-  
 04 3  
 0.24012136E-07-0.27494615E-11-0.23241445E+05 0.29017382E+02  
 4  
 R127C4H9O4UP C 4H 9O 4 G 0300.00 5000.00 1000.00  
 1  
 0.21226063E+02 0.18219627E-01-0.47519902E-05 0.62594929E-09-0.33771851E-  
 13 2  
 -0.28946961E+05-0.73806740E+02 0.12393204E+01 0.75103648E-01-0.62390653E-  
 04 3  
 0.24121507E-07-0.27879452E-11-0.23512396E+05 0.29048790E+02  
 4

R128C4H9O4UP C 4H 90 4 G 0300.00 5000.00 1000.00  
1  
0.20463877E+02 0.18947383E-01-0.50042804E-05 0.66612793E-09-0.36245394E-  
13 2  
-0.26179951E+05-0.69725555E+02 0.22620471E+01 0.67043088E-01-0.46687997E-  
04 3  
0.11577567E-07 0.84215762E-12-0.21034941E+05 0.24897638E+02  
4  
R129C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1  
0.24085417E+02 0.23195846E-01-0.63645057E-05 0.87288637E-09-0.48576699E-  
13 2  
-0.34966832E+05-0.88547226E+02 0.59372818E+00 0.90938896E-01-0.75367512E-  
04 3  
0.28450476E-07-0.28745201E-11-0.28674875E+05 0.32000023E+02  
4  
R130C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1  
0.22790810E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
13 2  
-0.31933617E+05-0.80004753E+02 0.65706697E+01 0.49368002E-01 0.18010354E-  
04 3  
-0.58097960E-07 0.25611062E-10-0.26736854E+05 0.81516495E+01  
4  
R131C3H7O2P C 3H 70 2 G 0300.00 5000.00 1000.00  
1  
0.13793248E+02 0.12478714E-01-0.30193419E-05 0.37854145E-09-0.19864939E-  
13 2  
-0.68557549E+04-0.39743660E+02 0.39244589E+00 0.56736656E-01-0.63722880E-  
04 3  
0.41441332E-07-0.11236257E-10-0.33718301E+04 0.28036133E+02  
4  
R132C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1  
0.22790564E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
13 2  
-0.31933396E+05-0.80695793E+02 0.65857382E+01 0.49265649E-01 0.18251547E-  
04 3  
-0.58334717E-07 0.25693662E-10-0.26738500E+05 0.73948445E+01  
4  
R133C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1  
0.22791502E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
13 2  
-0.31934242E+05-0.80701698E+02 0.65332913E+01 0.49625736E-01 0.17395208E-  
04 3  
-0.57487750E-07 0.25396334E-10-0.26732834E+05 0.76178002E+01  
4  
R134C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1  
0.22791945E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
13 2  
-0.32206387E+05-0.80703430E+02 0.65110831E+01 0.49780425E-01 0.17022903E-  
04 3  
-0.57115933E-07 0.25264783E-10-0.27002213E+05 0.77129507E+01  
4  
R135C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
1

0.22618525E+02 0.24565097E-01-0.68287231E-05 0.94424624E-09-0.52776732E-  
 13 2  
 -0.29731256E+05-0.78631691E+02 0.22531765E+01 0.77434152E-01-0.50057977E-  
 04 3  
 0.92221484E-08 0.23948675E-11-0.23949689E+05 0.27421509E+02  
 4  
 R136C5H11O4UP C 5H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.22790564E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
 13 2  
 -0.31933396E+05-0.80695908E+02 0.65857382E+01 0.49265649E-01 0.18251547E-  
 04 3  
 -0.58334717E-07 0.25693662E-10-0.26738500E+05 0.73947296E+01  
 4  
 R137C5H11O4UP C 5H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24084036E+02 0.23195846E-01-0.63645057E-05 0.87288637E-09-0.48576699E-  
 13 2  
 -0.34965582E+05-0.87846191E+02 0.66838330E+00 0.90424120E-01-0.74138872E-  
 04 3  
 0.27231698E-07-0.24456429E-11-0.28682904E+05 0.32375317E+02  
 4  
 R138C5H11O4UP C 5H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.24085417E+02 0.23195846E-01-0.63645057E-05 0.87288637E-09-0.48576699E-  
 13 2  
 -0.35238570E+05-0.87854149E+02 0.59372818E+00 0.90938896E-01-0.75367512E-  
 04 3  
 0.28450476E-07-0.28745201E-11-0.28946615E+05 0.32693100E+02  
 4  
 R139C5H11O4UP C 5H 11O 4 G 0300.00 5000.00 1000.00  
 1  
 0.22790810E+02 0.24664732E-01-0.68989102E-05 0.95939101E-09-0.53895243E-  
 13 2  
 -0.32205357E+05-0.80697960E+02 0.65706697E+01 0.49368002E-01 0.18010354E-  
 04 3  
 -0.58097960E-07 0.25611062E-10-0.27008594E+05 0.74584398E+01  
 4  
 R140C3H7O2P C 3H 7O 2 G 0300.00 5000.00 1000.00  
 1  
 0.14900070E+02 0.11743539E-01-0.28182487E-05 0.35167325E-09-0.18422740E-  
 13 2  
 -0.74383076E+04-0.46700554E+02-0.70671819E-01 0.60035869E-01-0.65301727E-  
 04 3  
 0.39138424E-07-0.96432836E-11-0.35576204E+04 0.29140375E+02  
 4  
 R141C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26957314E+02 0.25567064E-01-0.71132567E-05 0.98668584E-09-0.55402324E-  
 13 2  
 -0.45995523E+05-0.97023125E+02 0.19240208E+01 0.99853195E-01-0.88465495E-  
 04 3  
 0.39627178E-07-0.65964955E-11-0.39339785E+05 0.31045837E+02  
 4  
 R142C6H11O3KP C 6H 11O 3 G 0300.00 5000.00 1000.00  
 1  
 0.21269707E+02 0.25979394E-01-0.73657116E-05 0.10359127E-08-0.58725709E-  
 13 2

-0.31537477E+05-0.70252457E+02 0.25286846E+01 0.78772575E-01-0.62935869E-  
 04 3  
 0.27161263E-07-0.46660779E-11-0.26279527E+05 0.26641222E+02  
 4  
 R143C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26957314E+02 0.25567064E-01-0.71132567E-05 0.98668584E-09-0.55402324E-  
 13 2  
 -0.45995523E+05-0.96330116E+02 0.19240208E+01 0.99853195E-01-0.88465495E-  
 04 3  
 0.39627178E-07-0.65964955E-11-0.39339785E+05 0.31738844E+02  
 4  
 R144C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26960989E+02 0.25555488E-01-0.71065156E-05 0.98511632E-09-0.55275737E-  
 13 2  
 -0.45995469E+05-0.96347191E+02 0.20494347E+01 0.98976664E-01-0.86346285E-  
 04 3  
 0.37501639E-07-0.58416509E-11-0.39353102E+05 0.31208860E+02  
 4  
 R145C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26859884E+02 0.26164800E-01-0.73880888E-05 0.10341148E-08-0.58332516E-  
 13 2  
 -0.37172492E+05-0.96249313E+02 0.12120273E+01 0.99336259E-01-0.80679769E-  
 04 3  
 0.29436062E-07-0.26922024E-11-0.30253518E+05 0.35585342E+02  
 4  
 R146C4H7O3AP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.17457535E+02 0.14043124E-01-0.34465468E-05 0.43392298E-09-0.22686102E-  
 13 2  
 -0.18786379E+05-0.53121399E+02 0.12354443E+01 0.70066653E-01-0.83685976E-  
 04 3  
 0.56331743E-07-0.15482515E-10-0.14712065E+05 0.28265369E+02  
 4  
 R147C4H7O3AP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.17534180E+02 0.14827016E-01-0.38224639E-05 0.50040716E-09-0.26947379E-  
 13 2  
 -0.22133500E+05-0.56104538E+02 0.15593728E+01 0.66513143E-01-0.72171548E-  
 04 3  
 0.44645898E-07-0.11534675E-10-0.17953555E+05 0.24895702E+02  
 4  
 R148C4H7O3KP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.16971626E+02 0.14727856E-01-0.37093969E-05 0.47728843E-09-0.25398146E-  
 13 2  
 -0.24438244E+05-0.51118732E+02 0.27395420E+01 0.56707717E-01-0.53306736E-  
 04 3  
 0.29231964E-07-0.69305117E-11-0.20471291E+05 0.22153219E+02  
 4  
 R149C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26957314E+02 0.25567064E-01-0.71132567E-05 0.98668584E-09-0.55402324E-  
 13 2  
 -0.45995523E+05-0.97023048E+02 0.19240208E+01 0.99853195E-01-0.88465495E-  
 04 3

0.39627178E-07-0.65964955E-11-0.39339785E+05 0.31045914E+02  
 4  
 R150C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.27668777E+02 0.24906727E-01-0.68862546E-05 0.95102604E-09-0.53249211E-  
 13 2  
 -0.48736434E+05-0.10150513E+03 0.14391717E+01 0.10426346E+00-0.95663279E-  
 04 3  
 0.44007784E-07-0.74601115E-11-0.41875672E+05 0.32213806E+02  
 4  
 R151C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.27651623E+02 0.24939463E-01-0.69050616E-05 0.95539687E-09-0.53603308E-  
 13 2  
 -0.48730320E+05-0.10141097E+03 0.13948009E+01 0.10456868E+00-0.96390213E-  
 04 3  
 0.44727663E-07-0.77131097E-11-0.41870887E+05 0.32402214E+02  
 4  
 R152C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.27586744E+02 0.25481345E-01-0.71470799E-05 0.99521069E-09-0.55921942E-  
 13 2  
 -0.39920934E+05-0.10151276E+03 0.53830165E+00 0.10504944E+00-0.90985886E-  
 04 3  
 0.36895358E-07-0.46369132E-11-0.32769105E+05 0.36861099E+02  
 4  
 R153C3H5O3AP C 3H 5O 3 G 0300.00 5000.00 1000.00  
 1  
 0.15250555E+02 0.94761774E-02-0.21735109E-05 0.26085559E-09-0.13233574E-  
 13 2  
 -0.18536959E+05-0.45821560E+02 0.17292517E+01 0.55006772E-01-0.66182474E-  
 04 3  
 0.44485596E-07-0.12238302E-10-0.15055804E+05 0.22368870E+02  
 4  
 R154C3H5O3KP C 3H 5O 3 G 0300.00 5000.00 1000.00  
 1  
 0.14657055E+02 0.94415108E-02-0.21008623E-05 0.24607685E-09-0.12256772E-  
 13 2  
 -0.20831023E+05-0.40654873E+02 0.28928232E+01 0.45343868E-01-0.47697700E-  
 04 3  
 0.29476748E-07-0.77842160E-11-0.17572301E+05 0.19705057E+02  
 4  
 R155C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.27669922E+02 0.24906727E-01-0.68862546E-05 0.95102604E-09-0.53249211E-  
 13 2  
 -0.48737469E+05-0.10151080E+03 0.13795849E+01 0.10467589E+00-0.96650729E-  
 04 3  
 0.44989815E-07-0.78063892E-11-0.41869289E+05 0.32468174E+02  
 4  
 R156C6H11O5AUP C 6H 11O 5 G 0300.00 5000.00 1000.00  
 1  
 0.26957314E+02 0.25567064E-01-0.71132567E-05 0.98668584E-09-0.55402324E-  
 13 2  
 -0.45995523E+05-0.97023361E+02 0.19240208E+01 0.99853195E-01-0.88465495E-  
 04 3  
 0.39627178E-07-0.65964955E-11-0.39339785E+05 0.31045599E+02  
 4

R157C4H7O3AP C 4H 70 3 G 0300.00 5000.00 1000.00  
1  
0.17406540E+02 0.14109593E-01-0.34787290E-05 0.44083717E-09-0.23227559E-  
13 2  
-0.20633398E+05-0.52846531E+02 0.12384691E+01 0.70011266E-01-0.83759376E-  
04 3  
0.56577182E-07-0.15612527E-10-0.16572174E+05 0.28262407E+02  
4  
R158C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1  
0.27651623E+02 0.24939463E-01-0.69050616E-05 0.95539687E-09-0.53603308E-  
13 2  
-0.48458582E+05-0.10071789E+03 0.13948009E+01 0.10456868E+00-0.96390213E-  
04 3  
0.44727663E-07-0.77131097E-11-0.41599148E+05 0.33095299E+02  
4  
R159C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1  
0.27586744E+02 0.25481345E-01-0.71470799E-05 0.99521069E-09-0.55921942E-  
13 2  
-0.39649188E+05-0.10081969E+03 0.53830165E+00 0.10504944E+00-0.90985886E-  
04 3  
0.36895358E-07-0.46369132E-11-0.32497363E+05 0.37554180E+02  
4  
R160C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1  
0.27586744E+02 0.25481345E-01-0.71470799E-05 0.99521069E-09-0.55921942E-  
13 2  
-0.39649188E+05-0.10151276E+03 0.53830165E+00 0.10504944E+00-0.90985886E-  
04 3  
0.36895358E-07-0.46369132E-11-0.32497363E+05 0.36861099E+02  
4  
R161C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1  
0.27669472E+02 0.24906727E-01-0.68862546E-05 0.95102604E-09-0.53249211E-  
13 2  
-0.48465324E+05-0.10081604E+03 0.14018952E+01 0.10452050E+00-0.96276766E-  
04 3  
0.44616353E-07-0.76742605E-11-0.41599926E+05 0.33065578E+02  
4  
R162C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1  
0.27669922E+02 0.24906727E-01-0.68862546E-05 0.95102604E-09-0.53249211E-  
13 2  
-0.48737469E+05-0.10081772E+03 0.13795849E+01 0.10467589E+00-0.96650729E-  
04 3  
0.44989815E-07-0.78063892E-11-0.41869289E+05 0.33161259E+02  
4  
R163C3H5O3AP C 3H 50 3 G 0300.00 5000.00 1000.00  
1  
0.15042974E+02 0.89156954E-02-0.19267018E-05 0.22159319E-09-0.10946331E-  
13 2  
-0.17007553E+05-0.42112629E+02 0.14814140E+01 0.58020096E-01-0.76631637E-  
04 3  
0.55296169E-07-0.15923428E-10-0.13682696E+05 0.25435310E+02  
4  
R164C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
1



0.26957314E+02 0.25567064E-01-0.71132567E-05 0.98668584E-09-0.55402324E-  
 13 2  
 -0.45995523E+05-0.97023582E+02 0.19240208E+01 0.99853195E-01-0.88465495E-  
 04 3  
 0.39627178E-07-0.65964955E-11-0.39339785E+05 0.31045378E+02  
 4  
 R165C4H7O3AP C 4H 70 3 G 0300.00 5000.00 1000.00  
 1  
 0.18485838E+02 0.13420251E-01-0.32989458E-05 0.41840761E-09-0.22125993E-  
 13 2  
 -0.20932611E+05-0.59649029E+02 0.85003245E+00 0.72828628E-01-0.84293788E-  
 04 3  
 0.53367145E-07-0.13748593E-10-0.16494605E+05 0.29045883E+02  
 4  
 R166C5H11O2P C 5H 110 2 G 0300.00 5000.00 1000.00  
 1  
 0.18188122E+02 0.23514722E-01-0.65243621E-05 0.90092245E-09-0.50308390E-  
 13 2  
 -0.13984509E+05-0.59389362E+02 0.49283785E+00 0.76717511E-01-0.68574533E-  
 04 3  
 0.34870865E-07-0.74775854E-11-0.92142598E+04 0.31201130E+02  
 4  
 R167C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
 1  
 0.27585373E+02 0.25481345E-01-0.71470799E-05 0.99521069E-09-0.55921942E-  
 13 2  
 -0.47800168E+05-0.10150414E+03 0.61295676E+00 0.10453466E+00-0.89757239E-  
 04 3  
 0.35676582E-07-0.42080358E-11-0.40657609E+05 0.36544052E+02  
 4  
 R168C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
 1  
 0.27635616E+02 0.25388280E-01-0.70917290E-05 0.98200281E-09-0.54829713E-  
 13 2  
 -0.47819148E+05-0.10178110E+03 0.61498773E+00 0.10452989E+00-0.89769179E-  
 04 3  
 0.35711764E-07-0.42281196E-11-0.40657957E+05 0.36534645E+02  
 4  
 R169C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
 1  
 0.27634533E+02 0.25388280E-01-0.70917290E-05 0.98200281E-09-0.54829713E-  
 13 2  
 -0.48089891E+05-0.10177254E+03 0.66552615E+00 0.10417723E+00-0.88917099E-  
 04 3  
 0.34857063E-07-0.39244632E-11-0.40935074E+05 0.36322220E+02  
 4  
 R170C3H5O3AP C 3H 50 3 G 0300.00 5000.00 1000.00  
 1  
 0.16232840E+02 0.84770862E-02-0.18481044E-05 0.21291166E-09-0.10472056E-  
 13 2  
 -0.16448318E+05-0.50000000E+02 0.16590604E+00 0.61824515E-01-0.73026378E-  
 04 3  
 0.45571060E-07-0.11470842E-10-0.12376472E+05 0.30973866E+02  
 4  
 R171C6H11O5AUP C 6H 110 5 G 0300.00 5000.00 1000.00  
 1  
 0.26861605E+02 0.26164800E-01-0.73880888E-05 0.10341148E-08-0.58332516E-  
 13 2

-0.45326281E+05-0.96261963E+02 0.11242125E+01 0.99945955E-01-0.82145329E-  
 04 3  
 0.30899265E-07-0.32100069E-11-0.38396340E+05 0.35955982E+02  
 4  
 R172C4H7O3AP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.18532476E+02 0.13776614E-01-0.34525747E-05 0.44223045E-09-0.23439038E-  
 13 2  
 -0.74487988E+04-0.60375271E+02 0.70034224E-02 0.73230118E-01-0.78739708E-  
 04 3  
 0.45430880E-07-0.10652987E-10-0.26756191E+04 0.33445400E+02  
 4  
 R173C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10896326E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40122974E+02  
 4  
 R174C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10896340E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40122837E+02  
 4  
 R175C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10896339E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40122845E+02  
 4  
 R176C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.28831619E+02 0.26736606E-01-0.75019402E-05 0.10423002E-08-0.58337002E-  
 13 2  
 -0.76748445E+05-0.10637563E+03 0.27988429E+01 0.92994355E-01-0.50822284E-  
 04 3  
 -0.74667756E-08 0.11546110E-10-0.69598047E+05 0.28790094E+02  
 4  
 R177C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.19637131E+02 0.14397764E-01-0.35319665E-05 0.44722212E-09-0.23619329E-  
 13 2  
 -0.50335250E+05-0.63794151E+02-0.82991147E+00 0.88433526E-01-0.11112347E-  
 03 3  
 0.74046490E-07-0.19600108E-10-0.45506777E+05 0.37708191E+02  
 4  
 R178C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.19742794E+02 0.15128403E-01-0.38782182E-05 0.50716775E-09-0.27377001E-  
 13 2  
 -0.52682965E+05-0.67816055E+02-0.34758106E+00 0.83938129E-01-0.97486103E-  
 04 3

0.60301758E-07-0.14933435E-10-0.47762262E+05 0.32752544E+02  
 4  
 R179C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10896313E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40123100E+02  
 4  
 R180C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.30019293E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
 13 2  
 -0.80351242E+05-0.11313005E+03-0.55651587E+00 0.12214789E+00-0.12194804E-  
 03 3  
 0.60583424E-07-0.11180474E-10-0.72677844E+05 0.41359074E+02  
 4  
 R181C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.30019293E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
 13 2  
 -0.80351227E+05-0.11243695E+03-0.55651587E+00 0.12214789E+00-0.12194804E-  
 03 3  
 0.60583424E-07-0.11180474E-10-0.72677828E+05 0.42052170E+02  
 4  
 R182C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29032181E+02 0.26786620E-01-0.75428857E-05 0.10504563E-08-0.58875193E-  
 13 2  
 -0.79233938E+05-0.10721387E+03 0.70248280E+01 0.65551974E-01 0.15772855E-  
 04 3  
 -0.73338100E-07 0.34255938E-10-0.72647000E+05 0.10601790E+02  
 4  
 R183C3H5O4PB C 3H 5O 4 G 0300.00 5000.00 1000.00  
 1  
 0.17475679E+02 0.97410837E-02-0.22020317E-05 0.25982985E-09-0.12941161E-  
 13 2  
 -0.49091793E+05-0.56908089E+02-0.15645915E+00 0.72299726E-01-0.91204580E-  
 04 3  
 0.59867730E-07-0.15544798E-10-0.44867062E+05 0.30846706E+02  
 4  
 R184C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.30017719E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
 13 2  
 -0.80349797E+05-0.11311745E+03-0.47421721E+00 0.12157925E+00-0.12058653E-  
 03 3  
 0.59228288E-07-0.10702080E-10-0.72686688E+05 0.41012299E+02  
 4  
 R185C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10896345E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40122791E+02  
 4

R186C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
1  
0.19577709E+02 0.14474985E-01-0.35702080E-05 0.45551496E-09-0.24270044E-  
13 2  
-0.52177734E+05-0.63469776E+02-0.71370709E+00 0.87586373E-01-0.10928003E-  
03 3  
0.72365886E-07-0.19044790E-10-0.47378895E+05 0.37226894E+02  
4  
R187C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1  
0.30019293E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
13 2  
-0.80079484E+05-0.11313004E+03-0.55651587E+00 0.12214789E+00-0.12194804E-  
03 3  
0.60583424E-07-0.11180474E-10-0.72406086E+05 0.41359089E+02  
4  
R188C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1  
0.29032181E+02 0.26786620E-01-0.75428857E-05 0.10504563E-08-0.58875193E-  
13 2  
-0.78962188E+05-0.10790696E+03 0.70248280E+01 0.65551974E-01 0.15772855E-  
04 3  
-0.73338100E-07 0.34255938E-10-0.72375250E+05 0.99087076E+01  
4  
R189C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1  
0.28984154E+02 0.26875166E-01-0.75951366E-05 0.10628571E-08-0.59896607E-  
13 2  
-0.78943977E+05-0.10764169E+03 0.70599399E+01 0.65320507E-01 0.16300661E-  
04 3  
-0.73839828E-07 0.34425865E-10-0.72379180E+05 0.97583055E+01  
4  
R190C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1  
0.30018784E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
13 2  
-0.80079047E+05-0.11312592E+03-0.52637899E+00 0.12194318E+00-0.12146567E-  
03 3  
0.60109919E-07-0.11015275E-10-0.72409391E+05 0.41231564E+02  
4  
R191C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1  
0.30017719E+02 0.24961583E-01-0.68132667E-05 0.93025099E-09-0.51577608E-  
13 2  
-0.80349797E+05-0.11311745E+03-0.47421721E+00 0.12157925E+00-0.12058653E-  
03 3  
0.59228288E-07-0.10702080E-10-0.72686688E+05 0.41012299E+02  
4  
R192C3H5O4PB C 3H 5O 4 G 0300.00 5000.00 1000.00  
1  
0.17258120E+02 0.91939019E-02-0.19620195E-05 0.22196606E-09-0.10757545E-  
13 2  
-0.48567699E+05-0.53668056E+02-0.44616807E+00 0.75429201E-01-0.10176283E-  
03 3  
0.70702818E-07-0.19221810E-10-0.44492125E+05 0.33603085E+02  
4  
R193C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
1

0.29365206E+02 0.25513012E-01-0.69750581E-05 0.95034036E-09-0.52445072E-  
 13 2  
 -0.77631391E+05-0.10827059E+03-0.55248197E-01 0.11761460E+00-0.11443461E-  
 03 3  
 0.55870093E-07-0.10193776E-10-0.70143555E+05 0.40815643E+02  
 4  
 R194C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.20715464E+02 0.13674608E-01-0.33262452E-05 0.41803050E-09-0.21937726E-  
 13 2  
 -0.52497957E+05-0.71285988E+02-0.99640441E+00 0.89666151E-01-0.10803273E-  
 03 3  
 0.67368575E-07-0.16545675E-10-0.47312586E+05 0.36870071E+02  
 4  
 R195C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.28948002E+02 0.26949590E-01-0.76381966E-05 0.10729145E-08-0.60714502E-  
 13 2  
 -0.78932648E+05-0.10744689E+03 0.68298888E+01 0.66914387E-01 0.12476556E-  
 04 3  
 -0.70027575E-07 0.33078339E-10-0.72354539E+05 0.10732850E+02  
 4  
 R196C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.28982084E+02 0.26879052E-01-0.75975499E-05 0.10634258E-08-0.59942130E-  
 13 2  
 -0.78943242E+05-0.10762980E+03 0.70734167E+01 0.65233946E-01 0.16494008E-  
 04 3  
 -0.74021571E-07 0.34487271E-10-0.72380734E+05 0.97007761E+01  
 4  
 R197C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.28979372E+02 0.26879052E-01-0.75975499E-05 0.10634258E-08-0.59942130E-  
 13 2  
 -0.79212516E+05-0.10761039E+03 0.72153020E+01 0.64252898E-01 0.18842984E-  
 04 3  
 -0.76358802E-07 0.35311976E-10-0.72667711E+05 0.91007977E+01  
 4  
 R198C3H5O4PB C 3H 5O 4 G 0300.00 5000.00 1000.00  
 1  
 0.18078743E+02 0.92676291E-02-0.20761979E-05 0.24645558E-09-0.12498377E-  
 13 2  
 -0.47826211E+05-0.58731380E+02 0.12831578E+01 0.58628567E-01-0.50359879E-  
 04 3  
 0.15389210E-07 0.56307633E-12-0.43517336E+05 0.26877836E+02  
 4  
 R199C6H11O6UPB C 6H 11O 6 G 0300.00 5000.00 1000.00  
 1  
 0.28831030E+02 0.26737954E-01-0.75028879E-05 0.10425308E-08-0.58355637E-  
 13 2  
 -0.76748336E+05-0.10568020E+03 0.28153155E+01 0.92893407E-01-0.50609553E-  
 04 3  
 -0.76542666E-08 0.11605369E-10-0.69600008E+05 0.29410877E+02  
 4  
 R200C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.20395750E+02 0.14536544E-01-0.36682650E-05 0.47305271E-09-0.25230272E-  
 13 2

-0.80309658E+04-0.69202721E+02 0.13947588E+01 0.68191297E-01-0.51754112E-  
 04 3  
 0.11070645E-07 0.28092615E-11-0.30450325E+04 0.28198494E+02  
 4  
 R201C3H7O4UP C 3H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.18441828E+02 0.12571108E-01-0.29156811E-05 0.35375863E-09-0.18130491E-  
 13 2  
 -0.26782912E+05-0.62946449E+02 0.91786242E+00 0.56343596E-01-0.30807794E-  
 04 3  
 -0.52401790E-08 0.72193970E-11-0.21896840E+05 0.28333649E+02  
 4  
 R202C3H7O4UP C 3H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.18908276E+02 0.12915267E-01-0.31156469E-05 0.38901213E-09-0.20316124E-  
 13 2  
 -0.25335377E+05-0.64006973E+02 0.13388267E+01 0.64106293E-01-0.57643643E-  
 04 3  
 0.25205956E-07-0.39308422E-11-0.20607572E+05 0.26136774E+02  
 4  
 R203C3H7O2U C 3H 7O 2 G 0300.00 5000.00 1000.00  
 1  
 0.14195357E+02 0.13157809E-01-0.33661620E-05 0.43802198E-09-0.23482254E-  
 13 2  
 -0.13980988E+05-0.47413239E+02-0.38399315E+00 0.53882204E-01-0.45532583E-  
 04 3  
 0.19618367E-07-0.31824515E-11-0.98716543E+04 0.28052458E+02  
 4  
 R204C4H7O5AUP C 4H 7O 5 G 0300.00 5000.00 1000.00  
 1  
 0.22553045E+02 0.14503221E-01-0.35626765E-05 0.45021659E-09-0.23673549E-  
 13 2  
 -0.38854293E+05-0.76602470E+02 0.22920392E+01 0.76672606E-01-0.76092329E-  
 04 3  
 0.38896701E-07-0.78488856E-11-0.33548008E+05 0.26591852E+02  
 4  
 R205C4H7O5AUP C 4H 7O 5 G 0300.00 5000.00 1000.00  
 1  
 0.22507071E+02 0.14996783E-01-0.37708044E-05 0.48325460E-09-0.25571305E-  
 13 2  
 -0.30049473E+05-0.76801994E+02 0.15600102E+01 0.76306574E-01-0.68695241E-  
 04 3  
 0.29115421E-07-0.40960330E-11-0.24459779E+05 0.30521164E+02  
 4  
 R206C3H5O5AUP C 3H 5O 5 G 0300.00 5000.00 1000.00  
 1  
 0.20140787E+02 0.97907344E-02-0.21980736E-05 0.25930949E-09-0.12985304E-  
 13 2  
 -0.26420523E+05-0.66736542E+02 0.17457851E+01 0.64710304E-01-0.62509695E-  
 04 3  
 0.28765866E-07-0.47324883E-11-0.21564170E+05 0.27245560E+02  
 4  
 R207C4H7O5AUP C 4H 7O 5 G 0300.00 5000.00 1000.00  
 1  
 0.22145260E+02 0.14053375E-01-0.33048668E-05 0.40228554E-09-0.20506256E-  
 13 2  
 -0.40595742E+05-0.76559753E+02 0.19392399E+01 0.68454891E-01-0.48209342E-  
 04 3

0.74511419E-08 0.36396160E-11-0.35116559E+05 0.27804562E+02  
 4  
 R208C3H5O5AUP C 3H 50 5 G 0300.00 5000.00 1000.00  
 1  
 0.19680246E+02 0.90528997E-02-0.18644311E-05 0.20638653E-09-0.99123861E-  
 14 2  
 -0.36933332E+05-0.65267258E+02 0.20731230E+01 0.57213470E-01-0.42863128E-  
 04 3  
 0.79266469E-08 0.27150771E-11-0.32215324E+05 0.25442551E+02  
 4  
 R209C4H7O5AUP C 4H 70 5 G 0300.00 5000.00 1000.00  
 1  
 0.22553045E+02 0.14503221E-01-0.35626765E-05 0.45021659E-09-0.23673549E-  
 13 2  
 -0.38854293E+05-0.77295662E+02 0.22920392E+01 0.76672606E-01-0.76092329E-  
 04 3  
 0.38896701E-07-0.78488856E-11-0.33548008E+05 0.25898659E+02  
 4  
 R210C4H7O3AU C 4H 70 3 G 0300.00 5000.00 1000.00  
 1  
 0.17752764E+02 0.14889634E-01-0.38812755E-05 0.51236732E-09-0.27756629E-  
 13 2  
 -0.27464910E+05-0.59515358E+02 0.56896764E+00 0.66454582E-01-0.64002837E-  
 04 3  
 0.33332142E-07-0.71071209E-11-0.22812139E+05 0.28511850E+02  
 4  
 R211C4H7O3KP C 4H 70 3 G 0300.00 5000.00 1000.00  
 1  
 0.17661928E+02 0.14111058E-01-0.35076496E-05 0.44681342E-09-0.23604926E-  
 13 2  
 -0.27172420E+05-0.55486607E+02 0.21639087E+01 0.61751038E-01-0.62030740E-  
 04 3  
 0.35138942E-07-0.83346047E-11-0.22997527E+05 0.23705193E+02  
 4  
 R212C5H11O4UP C 5H 110 4 G 0300.00 5000.00 1000.00  
 1  
 0.22621819E+02 0.23870159E-01-0.64956016E-05 0.88758306E-09-0.49379751E-  
 13 2  
 -0.33794316E+05-0.81336517E+02 0.36972833E+01 0.58210768E-01 0.63013604E-  
 05 3  
 -0.51754320E-07 0.24379488E-10-0.28031035E+05 0.20090536E+02  
 4  
 R213C3H5O5AUP C 3H 50 5 G 0300.00 5000.00 1000.00  
 1  
 0.20137354E+02 0.97991768E-02-0.22026677E-05 0.26031574E-09-0.13062400E-  
 13 2  
 -0.34572113E+05-0.66719322E+02 0.16737509E+01 0.65207578E-01-0.63697873E-  
 04 3  
 0.29945316E-07-0.51476549E-11-0.29708639E+05 0.27550583E+02  
 4  
 R214C3H5O3AU C 3H 50 3 G 0300.00 5000.00 1000.00  
 1  
 0.15566469E+02 0.98117646E-02-0.23448367E-05 0.28927533E-09-0.14903902E-  
 13 2  
 -0.23004238E+05-0.50228695E+02-0.17706913E+00 0.55879112E-01-0.53762567E-  
 04 3  
 0.26558492E-07-0.51901994E-11-0.18687375E+05 0.30702753E+02  
 4

R215C4H7O5AUP                   C    4H    7O    5           G   0300.00   5000.00   1000.00  
1  
0.22479483E+02 0.15050177E-01-0.38016624E-05 0.49046245E-09-0.26157731E-  
13        2  
-0.38192043E+05-0.76652023E+02 0.14913710E+01 0.76787047E-01-0.69860442E-  
04        3  
0.30288994E-07-0.45146690E-11-0.32604705E+05 0.30810518E+02  
4  
R216C4H7O3AU                   C    4H    7O    3           G   0300.00   5000.00   1000.00  
1  
0.17722574E+02 0.15395133E-01-0.41242520E-05 0.55659244E-09-0.30674129E-  
13        2  
-0.18400754E+05-0.59822098E+02-0.36691189E+00 0.67496650E-01-0.59978847E-  
04        3  
0.26914917E-07-0.45464348E-11-0.13430257E+05 0.33304260E+02  
4  
R217C4H7O3KP                   C    4H    7O    3           G   0300.00   5000.00   1000.00  
1  
0.17696089E+02 0.14488758E-01-0.36731135E-05 0.47303278E-09-0.25082497E-  
13        2  
-0.26635014E+05-0.56142986E+02 0.13598177E+01 0.61881766E-01-0.55825098E-  
04        3  
0.26551895E-07-0.50086970E-11-0.22134244E+05 0.27939913E+02  
4  
R218C4H7O6UPB                   C    4H    7O    6           G   0300.00   5000.00   1000.00  
1  
0.24832123E+02 0.14693125E-01-0.35721212E-05 0.44835646E-09-0.23488915E-  
13        2  
-0.70442266E+05-0.88526566E+02 0.37532723E+00 0.94015002E-01-0.10109023E-  
03        3  
0.54202921E-07-0.11125023E-10-0.64358707E+05 0.34709370E+02  
4  
R219C4H7O6UPB                   C    4H    7O    6           G   0300.00   5000.00   1000.00  
1  
0.24435377E+02 0.15667506E-01-0.39533306E-05 0.50900051E-09-0.27077853E-  
13        2  
-0.69613945E+05-0.86698227E+02 0.27846887E+01 0.72421357E-01-0.44556444E-  
04        3  
-0.23079827E-08 0.82898549E-11-0.63764953E+05 0.25266901E+02  
4  
R220C3H5O6UPB                   C    3H    5O    6           G   0300.00   5000.00   1000.00  
1  
0.22125282E+02 0.10363654E-01-0.23268060E-05 0.27289410E-09-0.13520282E-  
13        2  
-0.66008047E+05-0.75559860E+02 0.28059280E+01 0.61936770E-01-0.40945713E-  
04        3  
-0.20521042E-09 0.68297299E-11-0.60851406E+05 0.24078405E+02  
4  
R221C4H7O6UPB                   C    4H    7O    6           G   0300.00   5000.00   1000.00  
1  
0.24437397E+02 0.14234310E-01-0.33188708E-05 0.40251263E-09-0.20525987E-  
13        2  
-0.72191156E+05-0.87869881E+02-0.80300272E-01 0.86504199E-01-0.74889751E-  
04        3  
0.24422070E-07-0.22139426E-12-0.65916156E+05 0.37051620E+02  
4  
R222C3H5O6UPB                   C    3H    5O    6           G   0300.00   5000.00   1000.00  
1



0.21994303E+02 0.92026955E-02-0.18655280E-05 0.20345080E-09-0.96413398E-  
 14 2  
 -0.68538547E+05-0.76702507E+02 0.20714929E-01 0.75496241E-01-0.70119662E-  
 04 3  
 0.25489348E-07-0.13613626E-11-0.63011480E+05 0.34828480E+02  
 4  
 R223C4H7O6UPB C 4H 7O 6 G 0300.00 5000.00 1000.00  
 1  
 0.24859968E+02 0.14640816E-01-0.35413811E-05 0.44106391E-09-0.22887586E-  
 13 2  
 -0.70452562E+05-0.88679756E+02 0.38100356E+00 0.93968242E-01-0.10095946E-  
 03 3  
 0.54054418E-07-0.11066629E-10-0.64359211E+05 0.34686371E+02  
 4  
 R224C4H7O4UB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.19990484E+02 0.15134205E-01-0.39023257E-05 0.51082161E-09-0.27501273E-  
 13 2  
 -0.59034977E+05-0.70507713E+02-0.14523062E+01 0.84506951E-01-0.90663256E-  
 04 3  
 0.50250819E-07-0.10936524E-10-0.53611445E+05 0.37768810E+02  
 4  
 R225C3H5O6UPB C 3H 5O 6 G 0300.00 5000.00 1000.00  
 1  
 0.22081966E+02 0.10442645E-01-0.23733853E-05 0.28394323E-09-0.14430077E-  
 13 2  
 -0.65991359E+05-0.76013161E+02 0.28456652E+01 0.61661191E-01-0.40283794E-  
 04 3  
 -0.86594670E-09 0.70636244E-11-0.60855660E+05 0.23216942E+02  
 4  
 R226C3H5O4UB C 3H 5O 4 G 0300.00 5000.00 1000.00  
 1  
 0.17397869E+02 0.10633072E-01-0.25918821E-05 0.32698963E-09-0.17244900E-  
 13 2  
 -0.54377559E+05-0.58882915E+02 0.88096887E+00 0.53093888E-01-0.32083473E-  
 04 3  
 -0.26365170E-08 0.64939378E-11-0.49821898E+05 0.26856810E+02  
 4  
 R227C4H7O6UPB C 4H 7O 6 G 0300.00 5000.00 1000.00  
 1  
 0.24435377E+02 0.15667506E-01-0.39533306E-05 0.50900051E-09-0.27077853E-  
 13 2  
 -0.69613945E+05-0.86005470E+02 0.27846887E+01 0.72421357E-01-0.44556444E-  
 04 3  
 -0.23079827E-08 0.82898549E-11-0.63764953E+05 0.25959658E+02  
 4  
 R228C4H7O4UB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.19615934E+02 0.16101956E-01-0.43097693E-05 0.58033489E-09-0.31884106E-  
 13 2  
 -0.57947809E+05-0.68817764E+02 0.99733800E+00 0.62626742E-01-0.33413624E-  
 04 3  
 -0.70125594E-08 0.87586752E-11-0.52750207E+05 0.28155413E+02  
 4  
 R229C3H7 C 3H 7O 0 G 0300.00 5000.00 1000.00  
 1  
 0.30132504E+01 0.22298312E-01-0.73345727E-05 0.11440690E-08-0.69462495E-  
 13 2

0.90991318E+04 0.10174383E+02 0.11280435E+01 0.28127538E-01-0.76147026E-  
 05 3  
 -0.74338771E-08 0.48445939E-11 0.93247773E+04 0.19138571E+02  
 4  
 R230C4H7O3AP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.18219597E+02 0.14222059E-01-0.36276433E-05 0.47176724E-09-0.25322565E-  
 13 2  
 -0.24866650E+05-0.60426842E+02 0.89012671E+00 0.72202682E-01-0.82437822E-  
 04 3  
 0.52081894E-07-0.13476424E-10-0.20469742E+05 0.26864763E+02  
 4  
 R231C4H7OA C 4H 7O 1 G 0300.00 5000.00 1000.00  
 1  
 0.12710145E+02 0.14461013E-01-0.38031676E-05 0.50663818E-09-0.27687842E-  
 13 2  
 -0.72049331E+04-0.36479786E+02 0.46037427E+00 0.53134870E-01-0.56684552E-  
 04 3  
 0.37296157E-07-0.10359909E-10-0.37958987E+04 0.26225351E+02  
 4  
 R232C3H5O3KP C 3H 5O 3 G 0300.00 5000.00 1000.00  
 1  
 0.15426951E+02 0.91295755E-02-0.20321866E-05 0.23623900E-09-0.11602229E-  
 13 2  
 -0.23046303E+05-0.45934586E+02 0.15084810E+01 0.50553318E-01-0.50311108E-  
 04 3  
 0.26903116E-07-0.59048309E-11-0.19234803E+05 0.25510868E+02  
 4  
 R233C3H5OA C 3H 5O 1 G 0300.00 5000.00 1000.00  
 1  
 0.10735343E+02 0.95132506E-02-0.23537664E-05 0.30050501E-09-0.15992739E-  
 13 2  
 -0.59952651E+04-0.30507957E+02 0.88138288E+00 0.38412623E-01-0.39839131E-  
 04 3  
 0.26051522E-07-0.73270574E-11-0.30714106E+04 0.20648191E+02  
 4  
 R234C4H7O3AP C 4H 7O 3 G 0300.00 5000.00 1000.00  
 1  
 0.17976183E+02 0.14210747E-01-0.35825171E-05 0.46045223E-09-0.24437222E-  
 13 2  
 -0.20599646E+05-0.57110531E+02 0.84427387E+00 0.68225279E-01-0.70501294E-  
 04 3  
 0.39307253E-07-0.88350846E-11-0.16118315E+05 0.29931089E+02  
 4  
 R235C4H7OA C 4H 7O 1 G 0300.00 5000.00 1000.00  
 1  
 0.12957436E+02 0.14907048E-01-0.40498171E-05 0.55197358E-09-0.30615775E-  
 13 2  
 -0.10572024E+05-0.40356571E+02-0.26849857E+00 0.56954298E-01-0.61621002E-  
 04 3  
 0.40629686E-07-0.11358460E-10-0.69331797E+04 0.27216013E+02  
 4  
 R236C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.20475136E+02 0.14434544E-01-0.36315082E-05 0.46619447E-09-0.24731021E-  
 13 2  
 -0.55433121E+05-0.71655632E+02-0.94260406E+00 0.89118645E-01-0.10654215E-  
 03 3

0.66540807E-07-0.16455066E-10-0.50286473E+05 0.35146809E+02  
 4  
 R237C4H7O2B C 4H 7O 2 G 0300.00 5000.00 1000.00  
 1  
 0.14888135E+02 0.14782420E-01-0.38427697E-05 0.50575277E-09-0.27313846E-  
 13 2  
 -0.38747836E+05-0.47123482E+02-0.15022156E+01 0.70767380E-01-0.82300729E-  
 04 3  
 0.53132496E-07-0.13790707E-10-0.34601320E+05 0.35239670E+02  
 4  
 R238C3H5O2B C 3H 5O 2 G 0300.00 5000.00 1000.00  
 1  
 0.12848969E+02 0.99354619E-02-0.24327853E-05 0.30600292E-09-0.16000825E-  
 13 2  
 -0.37557461E+05-0.40784027E+02-0.97244179E+00 0.55545449E-01-0.64522763E-  
 04 3  
 0.41097156E-07-0.10505753E-10-0.33944223E+05 0.29151291E+02  
 4  
 R239C4H7O4PB C 4H 7O 4 G 0300.00 5000.00 1000.00  
 1  
 0.19851742E+02 0.14957596E-01-0.37915840E-05 0.48989540E-09-0.26127355E-  
 13 2  
 -0.51989816E+05-0.66011604E+02 0.20080578E+01 0.64743347E-01-0.47263602E-  
 04 3  
 0.86949052E-08 0.32988120E-11-0.47264574E+05 0.25632217E+02  
 4  
 R240C4H7O2B C 4H 7O 2 G 0300.00 5000.00 1000.00  
 1  
 0.15098381E+02 0.15301439E-01-0.41333642E-05 0.56175598E-09-0.31137094E-  
 13 2  
 -0.41091355E+05-0.50945156E+02-0.21365950E+01 0.74134767E-01-0.86369393E-  
 04 3  
 0.55722222E-07-0.14553926E-10-0.36746590E+05 0.35638405E+02  
 4  
 R241C4H7O5AUP C 4H 7O 5 G 0300.00 5000.00 1000.00  
 1  
 0.23238993E+02 0.14303739E-01-0.35258067E-05 0.44278731E-09-0.22969282E-  
 13 2  
 -0.32799246E+05-0.82092857E+02 0.10253340E+01 0.81073180E-01-0.76774471E-  
 04 3  
 0.34399271E-07-0.52865711E-11-0.26990490E+05 0.31205624E+02  
 4  
 R242C4H7O5AUP C 4H 7O 5 G 0300.00 5000.00 1000.00  
 1  
 0.23240370E+02 0.14303739E-01-0.35258067E-05 0.44278731E-09-0.22969282E-  
 13 2  
 -0.40952707E+05-0.82100800E+02 0.95067888E+00 0.81587948E-01-0.78003111E-  
 04 3  
 0.35618054E-07-0.57154485E-11-0.35134672E+05 0.31523411E+02  
 4  
 R243C4H7O6UPB C 4H 7O 6 G 0300.00 5000.00 1000.00  
 1  
 0.25434103E+02 0.14645901E-01-0.36195097E-05 0.46023199E-09-0.24344772E-  
 13 2  
 -0.72507930E+05-0.92166756E+02-0.10238672E+01 0.99307537E-01-0.10384639E-  
 03 3  
 0.51707882E-07-0.92487832E-11-0.65938844E+05 0.41273796E+02  
 4

R244C4H7O6UPB                   C    4H    70    6           G   0300.00   5000.00   1000.00  
1  
0.25438341E+02 0.14638354E-01-0.36149995E-05 0.45916471E-09-0.24257682E-  
13    2  
-0.72509602E+05-0.92881699E+02-0.10258653E+01 0.99327147E-01-0.10390695E-  
03    3  
0.51780958E-07-0.92786915E-11-0.65938711E+05 0.40590092E+02  
4  
R245C5H9OA                    C    5H    90    1           G   0300.00   5000.00   1000.00  
1  
0.15357846E+02 0.19727506E-01-0.55181363E-05 0.76757489E-09-0.43138477E-  
13    2  
-0.98249580E+04-0.48975994E+02-0.47400647E+00 0.69105305E-01-0.69549824E-  
04    3  
0.42165098E-07-0.10954920E-10-0.55051328E+04 0.31953388E+02  
4  
R246C5H9O2B                   C    5H    90    2           G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13    2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04    3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
RC3H5Y                         C    3H    50    0           G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13    2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04    3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
RC4H7Y                         C    4H    70    0           G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13    2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04    3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
RC3H5O                         C    3H    50    1           G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13    2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04    3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
RC5H9O                         C    5H    90    1           G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13    2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04    3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
RC5H9Y                         C    5H    90    0           G   0300.00   5000.00   1000.00  
1

0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC6H9OZ C 6H 90 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC5H7OZ C 5H 70 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC4H5OZ C 4H 50 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC3H5O3 C 3H 50 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC5H9O3 C 5H 90 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC6H9O3Z C 6H 90 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC5H7O3Z C 5H 70 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2

-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC4H5O3Z C 4H 50 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC7H130 C 7H 130 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC6H13 C 6H 130 0 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 RC7H1303 C 7H 130 3 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 C5H9OE#4 C 5H 90 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 C5H9OE#5 C 5H 90 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3  
 0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
 4  
 C5H9OE#6 C 5H 90 1 G 0300.00 5000.00 1000.00  
 1  
 0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
 13 2  
 -0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
 04 3

0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#4U C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#5U C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#6U C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#4P C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#5P C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O3E#6P C 5H 90 3 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O5E#4UP C 5H 90 5 G 0300.00 5000.00 1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13 2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04 3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4

C5H9O5E#5UP                    C   5H   90   5        G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13     2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04     3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
C5H9O5E#6UP                    C   5H   90   5        G   0300.00   5000.00   1000.00  
1  
0.17552582E+02 0.20030502E-01-0.55556238E-05 0.76777634E-09-0.42941223E-  
13     2  
-0.41376172E+05-0.59720062E+02-0.25150366E+01 0.87286346E-01-0.96496748E-  
04     3  
0.59345126E-07-0.14867392E-10-0.36302215E+05 0.41297184E+02  
4  
!Added Thermo  
R290C6H11O3AU                  C   6H   110   3        G   0300.00   5000.00   1000.00  
1  
-0.31873410E+01 0.66592187E-01-0.26575746E-04 0.47471835E-08-0.31663943E-  
12     2  
-0.31931262E+05 0.60965408E+02-0.30994337E+01 0.94740964E-01-0.76125056E-  
04     3  
0.27519651E-07-0.18483093E-11-0.34963906E+05 0.49776138E+02  
4  
R291C6H11O3AP                  C   6H   110   3        G   0300.00   5000.00   1000.00  
1  
-0.20556655E+01 0.63473053E-01-0.24790130E-04 0.43615103E-08-0.28781356E-  
12     2  
-0.26214135E+05 0.59070667E+02-0.28774247E+01 0.10249678E+00-0.10239673E-  
03     3  
0.54318836E-07-0.10889737E-10-0.29404318E+05 0.50524788E+02  
4  
R292C6H11O3AP                  C   6H   110   3        G   0300.00   5000.00   1000.00  
1!as R291  
-0.20556655E+01 0.63473053E-01-0.24790130E-04 0.43615103E-08-0.28781356E-  
12     2  
-0.26214135E+05 0.59070667E+02-0.28774247E+01 0.10249678E+00-0.10239673E-  
03     3  
0.54318836E-07-0.10889737E-10-0.29404318E+05 0.50524788E+02  
4  
R293C6H11O3AP                  C   6H   110   3        G   0300.00   5000.00   1000.00  
1!as R291  
-0.24133644E+01 0.64190999E-01-0.25175190E-04 0.44428434E-08-0.29384500E-  
12     2  
-0.26127568E+05 0.60934158E+02-0.18565714E+01 0.95248930E-01-0.86116110E-  
04     3  
0.39381103E-07-0.59491041E-11-0.29503203E+05 0.46268227E+02  
4  
R300C6H11O5APU                 C   6H   110   5        G   0300.00   5000.00   1000.00  
1  
-0.38794198E+01 0.75715631E-01-0.30846310E-04 0.55898006E-08-0.37662115E-  
12     2  
-0.43560375E+05 0.74186981E+02-0.14545058E+01 0.10642760E+00-0.87977714E-  
04     3  
0.29609220E-07-0.49951953E-12-0.48277746E+05 0.47314251E+02  
4



R301C6H11O5APU C 6H 11O 5 G 0300.00 5000.00 1000.00  
1!same as R300  
-0.38794198E+01 0.75715631E-01-0.30846310E-04 0.55898006E-08-0.37662115E-  
12 2  
-0.43560375E+05 0.74186981E+02-0.14545058E+01 0.10642760E+00-0.87977714E-  
04 3  
0.29609220E-07-0.49951953E-12-0.48277746E+05 0.47314251E+02  
4  
R302C6H11O5APU C 6H 11O 5 G 0300.00 5000.00 1000.00  
1!same as R300  
-0.38794198E+01 0.75715631E-01-0.30846310E-04 0.55898006E-08-0.37662115E-  
12 2  
-0.43560375E+05 0.74186981E+02-0.14545058E+01 0.10642760E+00-0.87977714E-  
04 3  
0.29609220E-07-0.49951953E-12-0.48277746E+05 0.47314251E+02  
4  
R305C6H11O5APP C 6H 11O 5 G 0300.00 5000.00 1000.00  
1  
-0.30903029E+01 0.73255107E-01-0.29389392E-04 0.52693663E-08-0.35240108E-  
12 2  
-0.37756844E+05 0.73397766E+02-0.40634668E+00 0.10829552E+00-0.10125590E-  
03 3  
0.44768729E-07-0.57723548E-11-0.42796352E+05 0.43939034E+02  
4  
R306C6H11O5APP C 6H 11O 5 G 0300.00 5000.00 1000.00  
1!as R305  
-0.30903029E+01 0.73255107E-01-0.29389392E-04 0.52693663E-08-0.35240108E-  
12 2  
-0.37756844E+05 0.73397766E+02-0.40634668E+00 0.10829552E+00-0.10125590E-  
03 3  
0.44768729E-07-0.57723548E-11-0.42796352E+05 0.43939034E+02  
4  
R307C6H11O5APP C 6H 11O 5 G 0300.00 5000.00 1000.00  
1!as R305  
-0.30903029E+01 0.73255107E-01-0.29389392E-04 0.52693663E-08-0.35240108E-  
12 2  
-0.37756844E+05 0.73397766E+02-0.40634668E+00 0.10829552E+00-0.10125590E-  
03 3  
0.44768729E-07-0.57723548E-11-0.42796352E+05 0.43939034E+02  
4  
R310C6H11O7APPU C 6H 11O 7 G 0300.00 5000.00 1000.00  
1  
-0.50275264E+01 0.85672483E-01-0.35590103E-04 0.65388823E-08-0.44491743E-  
12 2  
-0.55288824E+05 0.89239319E+02-0.99669695E-01 0.12009586E+00-0.10450054E-  
03 3  
0.36258538E-07-0.72615004E-12-0.61831891E+05 0.45394489E+02  
4  
R311C6H11O7APPU C 6H 11O 7 G 0300.00 5000.00 1000.00  
1!as R310  
-0.50275264E+01 0.85672483E-01-0.35590103E-04 0.65388823E-08-0.44491743E-  
12 2  
-0.55288824E+05 0.89239319E+02-0.99669695E-01 0.12009586E+00-0.10450054E-  
03 3  
0.36258538E-07-0.72615004E-12-0.61831891E+05 0.45394489E+02  
4  
R312C6H11O7APPU C 6H 11O 7 G 0300.00 5000.00 1000.00  
1!as R310

-0.50275264E+01 0.85672483E-01-0.35590103E-04 0.65388823E-08-0.44491743E-  
 12 2  
 -0.55288824E+05 0.89239319E+02-0.99669695E-01 0.12009586E+00-0.10450054E-  
 03 3  
 0.36258538E-07-0.72615004E-12-0.61831891E+05 0.45394489E+02  
 4  
 C6H8OK(OOH)2O C 6H 100 6 G 0300.00 5000.00 1000.00  
 1  
 -0.23686100E+02 0.11349288E+00-0.52927953E-04 0.10556365E-07-0.76221001E-  
 12 2  
 -0.69050984E+05 0.18851312E+03-0.17706923E+01 0.10867160E+00-0.89435496E-  
 04 3  
 0.26851414E-07 0.20178843E-11-0.81016352E+05 0.54075203E+02  
 4  
 C6H11OKOOH C 6H 120 3 G 0300.00 5000.00 1000.00  
 1  
 -0.56812325E+01 0.74481487E-01-0.31313215E-04 0.58010134E-08-0.39701456E-  
 12 2  
 -0.48854383E+05 0.75975227E+02-0.16661570E+01 0.90130769E-01-0.63648586E-  
 04 3  
 0.16118886E-07 0.18379686E-11-0.52942109E+05 0.44760433E+02  
 4  
 gcaprolac C 6H 100 2 G 0300.00 5000.00 1000.00  
 1  
 -0.39845737E+02 0.12860426E+00-0.63139865E-04 0.13068464E-07-0.96981949E-  
 12 2  
 -0.39214703E+05 0.25324310E+03-0.91122885E+01 0.10346702E+00-0.86667511E-  
 04 3  
 0.28211613E-07 0.12123542E-11-0.53759207E+05 0.72251762E+02  
 4  
 dcaprolac C 6H 100 2 G 0300.00 5000.00 1000.00  
 1 !thermo wrong  
 -0.39845737E+02 0.12860426E+00-0.63139865E-04 0.13068464E-07-0.96981949E-  
 12 2  
 -0.39214703E+05 0.25324310E+03-0.91122885E+01 0.10346702E+00-0.86667511E-  
 04 3  
 0.28211613E-07 0.12123542E-11-0.53759207E+05 0.72251762E+02  
 4  
  
 C6H12OOHP C 6H 130 3 G 0300.00 5000.00 1000.00  
 1  
 0.40406521E+02 0.43155509E-02-0.33395790E-06 0.13614016E-10-0.14257149E-  
 15 2  
 -0.43256535E+05-0.18384412E+03-0.71287930E+00 0.87393552E-01-0.54166787E-  
 04 3  
 0.13415186E-07-0.15294423E-11-0.28776391E+05 0.39952187E+02  
 4  
 HCOOOH C 1H 20 3 G 0300.00 5000.00 1000.00  
 1  
 0.84613352E+01 0.64787990E-02-0.22582392E-05 0.36714173E-09-0.22947380E-  
 13 2  
 -0.69612359E+05-0.15757065E+02 0.38585081E+01 0.18375801E-01-0.11974998E-  
 04 3  
 0.24552156E-08 0.30738495E-12-0.68307195E+05 0.82209072E+01  
 4  
 C6H11OKOH C 6H 130 2 G 0300.00 5000.00 1000.00  
 1

0.37551144E+02 0.46787024E-02-0.42779283E-06 0.27691910E-10-0.11117922E-  
14 2  
-0.50672633E+05-0.17236607E+03-0.19853777E+01 0.82333386E-01-0.47971320E-  
04 3  
0.10505519E-07-0.10552669E-11-0.36524238E+05 0.43630539E+02

4  
HCOOH C 1H 2O 2 G 0300.00 5000.00 1000.00  
1

0.45464592E+01 0.80251126E-02-0.30039655E-05 0.51283428E-09-0.33126418E-  
13 2  
-0.47485980E+05 0.11247597E+01 0.14237809E+01 0.16171511E-01-0.96905951E-  
05 3  
0.19028237E-08 0.23235068E-12-0.46608219E+05 0.17362677E+02

4  
C6H11OKO C 6H 11O 2 G 0300.00 5000.00 1000.00  
1

-0.25180285E+01 0.61358701E-01-0.24090034E-04 0.42542228E-08-0.28148889E-  
12 2  
-0.33437289E+05 0.52939030E+02-0.12126077E+01 0.80570221E-01-0.56666246E-  
04 3  
0.14181447E-07 0.17820504E-11-0.36384246E+05 0.37173130E+02

4

!Thermo for 1-hexanol derived species

C6H14OL-1 C 6H 14O 1 G 0300.00 5000.00 1000.00  
1

0.12937091E+02 0.40724754E-01-0.14038817E-04 0.22635591E-08-0.14061088E-  
12 2  
-0.45116164E+05-0.34646095E+02 0.17089731E+01 0.62823847E-01-0.15247690E-  
04 3  
-0.17000842E-07 0.94616892E-11-0.41638996E+05 0.25441233E+02

4  
C6H12OLZ C 6H 12O 1 G 0300.00 5000.00 1000.00  
1

0.12660265E+02 0.36133874E-01-0.12532662E-04 0.20306372E-08-0.12663294E-  
12 2  
-0.30159793E+05-0.34224583E+02-0.76489490E+00 0.70599921E-01-0.36976613E-  
04 3  
0.88159086E-09 0.44254773E-11-0.26442834E+05 0.35514053E+02

4

R32C6H13OL C 6H 13O 1 G 0300.00 5000.00 1000.00  
1

0.16804916E+02 0.30745033E-01-0.91333513E-05 0.13269967E-08-0.76844679E-  
13 2  
-0.24704252E+05-0.53686958E+02 0.12100586E+01 0.70196413E-01-0.43787499E-  
04 3  
0.13029002E-07-0.98122443E-12-0.20028326E+05 0.28239624E+02

4  
R33C6H13O C 6H 13O 1 G 0300.00 5000.00 1000.00  
1

0.16690638E+02 0.31916361E-01-0.97278480E-05 0.14366939E-08-0.83977245E-  
13 2  
-0.20339602E+05-0.56680149E+02-0.12510051E+01 0.76089367E-01-0.43349803E-  
04 3  
0.63367391E-08 0.24065680E-11-0.15000264E+05 0.37638317E+02

4

R34C6H13OL                    C    6H   130    1        G   0300.00    5000.00   1000.00  
1  
0.17426226E+02 0.30211745E-01-0.89496298E-05 0.12969930E-08-0.74939058E-  
13        2  
-0.21957279E+05-0.57300301E+02 0.43363652E+00 0.74804127E-01-0.50843028E-  
04        3  
0.17779378E-07-0.22637200E-11-0.16979256E+05 0.31487730E+02  
4  
R35C6H13OL                    C    6H   130    1        G   0300.00    5000.00   1000.00  
1  
0.16893269E+02 0.30602524E-01-0.90562389E-05 0.13094720E-08-0.75434193E-  
13        2  
-0.22869385E+05-0.54163818E+02 0.13819655E+01 0.69038518E-01-0.40799303E-  
04        3  
0.98736708E-08 0.17874062E-12-0.18186941E+05 0.27501730E+02  
4  
R36C6H13OL                    C    6H   130    1        G   0300.00    5000.00   1000.00  
1  
0.17110497E+02 0.30166524E-01-0.88625357E-05 0.12747101E-08-0.73162478E-  
13        2  
-0.22903615E+05-0.55257992E+02 0.39506140E+00 0.76039314E-01-0.56460191E-  
04        3  
0.24169763E-07-0.45279167E-11-0.18091504E+05 0.31616184E+02  
4  
R37C6H13OL                    C    6H   130    1        G   0300.00    5000.00   1000.00  
1  
0.17110497E+02 0.30166524E-01-0.88625357E-05 0.12747101E-08-0.73162478E-  
13        2  
-0.22903615E+05-0.55257992E+02 0.39506140E+00 0.76039314E-01-0.56460191E-  
04        3  
0.24169763E-07-0.45279167E-11-0.18091504E+05 0.31616184E+02  
4  
R38C6H13OL                    C    6H   130    1        G   0300.00    5000.00   1000.00  
1  
0.17110497E+02 0.30166524E-01-0.88625357E-05 0.12747101E-08-0.73162478E-  
13        2  
-0.22903615E+05-0.55257992E+02 0.39506140E+00 0.76039314E-01-0.56460191E-  
04        3  
0.24169763E-07-0.45279167E-11-0.18091504E+05 0.31616184E+02  
4  
R51C6H13O3LU                    C    6H   130    3        G   0300.00    5000.00   1000.00  
1  
0.21665171E+02 0.30368604E-01-0.87223625E-05 0.12321352E-08-0.69733207E-  
13        2  
-0.36119199E+05-0.77376091E+02 0.22206380E+01 0.64930715E-01 0.56954314E-  
05        3  
-0.53491341E-07 0.25118371E-10-0.30118404E+05 0.27115112E+02  
4  
R53C4H9OL                    C    4H    90    1        G   0300.00    5000.00   1000.00  
1  
0.13425339E+02 0.18552562E-01-0.50860740E-05 0.69812223E-09-0.38928408E-  
13        2  
-0.14622205E+05-0.40021164E+02-0.87729210E+00 0.61106708E-01-0.55880286E-  
04        3  
0.30374938E-07-0.71730477E-11-0.10657623E+05 0.33512131E+02  
4  
R55C3H7OL                    C    3H    70    1        G   0300.00    5000.00   1000.00  
1

0.11141162E+02 0.13060917E-01-0.33221684E-05 0.43202319E-09-0.23235532E-  
13 2  
-0.11349815E+05-0.29429979E+02 0.98580189E-01 0.45494240E-01-0.43997876E-  
04 3  
0.27192735E-07-0.74989806E-11-0.81603545E+04 0.27702703E+02  
4

R302C6H13 C 6H 130 0 G 0300.00 5000.00 1000.00  
1  
0.13832993E+02 0.32867298E-01-0.10277109E-04 0.15470342E-08-0.91690083E-  
13 2  
-0.22547227E+04-0.42393444E+02-0.60901982E+00 0.72525367E-01-0.47735059E-  
04 3  
0.14527513E-07-0.83027671E-12 0.17468357E+04 0.32297169E+02  
4

R303C5H11OL C 5H 110 1 G 0300.00 5000.00 1000.00  
1  
0.15492600E+02 0.24319727E-01-0.69868101E-05 0.99109565E-09-0.56465158E-  
13 2  
-0.18138992E+05-0.49128529E+02-0.84957099E+00 0.71238436E-01-0.58610531E-  
04 3  
0.27361477E-07-0.53796629E-11-0.13576224E+05 0.35193016E+02  
4

END

REACTIONS

! 1498 reactions

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

! molecular elimination :  
! unimolecular initiations :

!n-pentane

C5H12-1=R11C2H5+R19C3H7 1.9E+0017 0.000 86072.0 ! UI 1 KB

C5H12-1=R4CH3+R20C4H9 4.1E+0017 0.000 87589.3 ! UI 2 KB

!hexanal

C6H12OA-1=R27C5H11+R5CHO 4.3E+0016 0.000 82121.6 ! UI 3 KB

C6H12OA-1=R20C4H9+R13CH2CHO 3.1E+0016 0.000 83390.5 ! UI 4 KB

C6H12OA-1=R19C3H7+R49C3H5OA 9.2E+0016 0.000 86794.6 ! UI 5 KB

C6H12OA-1=R11C2H5+R47C4H7OA 7.8E+0016 0.000 86034.8 ! UI 6 KB

C6H12OA-1=R4CH3+R245C5H9OA 1.5E+0017 0.000 87155.2 ! UI 7 KB

!hexanoic acid

C6H12O2B-1=R2OH+R29C6H11OK 1.5E+0017 0.000 106324.2 ! UI 8 KB

C6H12O2B-1=R1H+R35C6H11O2K 2.3E+0014 0.000 106345.2 ! UI 9 KB

C6H12O2B-1=R27C5H11+R22CO2H 8.6E+0016 0.000 88540.3 ! UI 10 KB

C6H12O2B-1=R20C4H9+R23C2H3O2B 3.8E+0016 0.000 79324.4 ! UI 11 KB

C6H12O2B-1=R19C3H7+R56C3H5O2B 1.0E+0017 0.000 87301.4 ! UI 12 KB

C6H12O2B-1=R11C2H5+R54C4H7O2B 8.6E+0016 0.000 86541.6 ! UI 13 KB

C6H12O2B-1=R4CH3+R246C5H9O2B 1.7E+0017 0.000 87662.0 ! UI 14 KB

!1-hexanol

C6H14OL-1=R2OH+R302C6H13 1.2E+0016 0.000 94913.9 ! UI 7 KB

C6H14OL-1=R1H+R33C6H13O 1.7E+0014 0.000 104497.5 ! UI 8 KB

C6H14OL-1=R27C5H11+R6CH2OH 6.9E+0016 0.000 87738.1 ! UI 9 KB

C6H14OL-1=R20C4H9+R24C2H4OH 1.1E+0017 0.000 87724.8 ! UI 10 KB

C6H14OL-1=R19C3H7+R55C3H7OL 1.1E+0017 0.000 87354.6 ! UI 11 KB

C6H14OL-1=R11C2H5+R53C4H9OL 7.7E+0016 0.000 87288.1 ! UI 12 KB  
C6H14OL-1=R4CH3+R303C5H11OL 1.5E+0017 0.000 88409.1 ! UI 13 KB

! bimolecular initiations :

!n-pentane

C5H12-1+O2=R3OOH+R26C5H11 1.4E+0013 0.000 50652.7 ! BI 15 CN  
C5H12-1+O2=R3OOH+R27C5H11 4.2E+0013 0.000 53034.7 ! BI 16 CN  
C5H12-1+O2=R3OOH+R28C5H11 2.8E+0013 0.000 50589.9 ! BI 17 CN

!hexanal

C6H12OA-1+O2=R3OOH+R29C6H11OK 7.0E+0012 0.000 38995.0 ! BI 18 CN  
C6H12OA-1+O2=R3OOH+R30C6H11OA 2.1E+0013 0.000 52522.6 ! BI 19 CN  
C6H12OA-1+O2=R3OOH+R31C6H11OA 1.4E+0013 0.000 50078.7 ! BI 20 CN  
C6H12OA-1+O2=R3OOH+R32C6H11OA 1.4E+0013 0.000 50141.6 ! BI 21 CN  
C6H12OA-1+O2=R3OOH+R33C6H11OA 1.4E+0013 0.000 50141.6 ! BI 22 CN  
C6H12OA-1+O2=R3OOH+R34C6H11OA 1.4E+0013 0.000 43995.2 ! BI 23 CN

!Olive

!2C6H12OA-1=R32C6H13OL+R29C6H11OK 1.9E+0014 0.000 53000.0

!hexanoic acid

C6H12O2B-1+O2=R3OOH+R35C6H11O2K 7.0E+0012 0.000 57766.1 ! BI 24 CN  
C6H12O2B-1+O2=R3OOH+R36C6H11O2B 2.1E+0013 0.000 53029.4 ! BI 25 CN  
C6H12O2B-1+O2=R3OOH+R37C6H11O2B 1.4E+0013 0.000 50585.5 ! BI 26 CN  
C6H12O2B-1+O2=R3OOH+R38C6H11O2B 1.4E+0013 0.000 50648.4 ! BI 27 CN  
C6H12O2B-1+O2=R3OOH+R39C6H11O2B 1.4E+0013 0.000 50648.4 ! BI 28 CN  
C6H12O2B-1+O2=R3OOH+R40C6H11O2B 1.4E+0013 0.000 46509.1 ! BI 29 CN

!1-hexanol

!C6H14OL-1+O2=R3OOH+R32C6H13OL 1.4E+0013 0.000 46869.1 ! BI 22 CN  
C6H14OL-1+O2=R3OOH+R33C6H13O 7.0E+0012 0.000 55918.6 ! BI 23 CN  
C6H14OL-1+O2=R3OOH+R34C6H13OL 2.1E+0013 0.000 53033.0 ! BI 24 CN  
C6H14OL-1+O2=R3OOH+R35C6H13OL 1.4E+0013 0.000 50588.2 ! BI 25 CN  
C6H14OL-1+O2=R3OOH+R36C6H13OL 1.4E+0013 0.000 50652.5 ! BI 26 CN  
C6H14OL-1+O2=R3OOH+R37C6H13OL 1.4E+0013 0.000 50652.5 ! BI 27 CN  
C6H14OL-1+O2=R3OOH+R38C6H13OL 1.4E+0013 0.000 50652.5 ! BI 28 CN

! additions :

!Olive: additions to the carbonyl group

!H additions to hexanal

R32C6H13OL=R1H+C6H12OA-1 2.5E+0013 0.000 29000.0 ! DE 757 CN  
R33C6H13O=R1H+C6H12OA-1 2.4E+0013 0.000 20900.0 ! DE 760  
R32C6H13OL+O2=R51C6H13O3LU 1.0E+0019 -2.500 0.0 ! ADO 39 CN  
R51C6H13O3LU=C6H12O2B-1+R2OH 9.9E+0007 1.000 22000.0 ! IS 206 KB  
duplicate  
R51C6H13O3LU=C6H12O2B-1+R2OH 1.7E+0007 1.000 21000.0 ! IS 207 KB  
duplicate  
R51C6H13O3LU=>C6H12O2B-1+R2OH 3.98e12 0.000 37100.0!Olive  
duplicate

!6H12OA-1+B1O=>C6H12O2B-1

6.0E+004 2.56 -1130.0

!C6H12OA-1+R2OH=>C6H11OKOH

6.32E+006 1.630 4284.0 !addition

of OH (model is CH2O, Xu et al., 2006 IJCK)

C6H12OA-1+R2OH=C6H11OKOH

1.13E+5 2.28 -2466 !

!C6H12OA-1+R2OH=>C6H11OKOH

5.65E+5 2.28 -2466 !Olive A\*5

C6H11OKOH=HCOOH+R27C5H11

4.45E+014 -0.220 27200.0 !b-

scission C-C

C6H11OKOH=C6H12O2B-1+R1H

5.00E+013 0.000 21900.0 !b-

scission C-H

C6H11OKOH+O2=C6H12O2B-1+R3OOH

6.03E+010 0.000 1649.0 !oxidation

C6H12OA-1+R3OOH=>C6H12OOHP

1.05E+012 0.000 13100.0 !addition

of HO2

```

C6H12OOHP=>C6H11OKOOH+R1H          5.00E+013  0.000  21900.0  !b-
scission C-H
C6H12OOHP+O2=>C6H11OKOOH+R3OOH      6.03E+010  0.000   1649.0
!oxidation
C6H12OOHP=>R27C5H11+HCOOOH          4.45E+014 -0.220  27200.0  !b-
scission C-C
HCOOOH=R2OH+CO2+R1H                 1.00E+016  0.000   40.0E3
!(406)<CAVANAGH90>!
!
! Ipso-additions :

! additions with oxygen:
R19C3H7+O2=R41C3H7O2U          9.0E+0018 -2.500  0.0  ! ADO 30 CN
R20C4H9+O2=R42C4H9O2U          9.0E+0018 -2.500  0.0  ! ADO 31 CN
R26C5H11+O2=R43C5H11O2U        1.8E+0019 -2.500  0.0  ! ADO 32 CN
R27C5H11+O2=R44C5H11O2U        18.0E+0018 -2.500  0.0  ! ADO 33 CN 9.0E+0018
R28C5H11+O2=R45C5H11O2U        3.4E+0019 -2.500  0.0  ! ADO 34 CN 1.7E+0019
!
!Olive: missing addition to O2 for R29C6H11OK
!R29C6H11OK+O2=R290C6H11O3AU          2.84E+07   2.37  384.0 !Hou
et al., 2005, theory
R29C6H11OK+O2=R290C6H11O3AU          1.8E+0019 -2.500  0.0  !
!R29C6H11OK+O2=R290C6H11O3AU          3.6E+0019 -2.500  0.0
R291C6H11O3AP+O2=R300C6H11O5APU      1.8E+0019 -2.500  0.0  !
R292C6H11O3AP+O2=R301C6H11O5APU      1.8E+0019 -2.500  0.0  !
R293C6H11O3AP+O2=R302C6H11O5APU      1.8E+0019 -2.500  0.0  !
R305C6H11O5APP+O2=R310C6H11O7APPU     1.8E+0019 -2.500  0.0  !
R306C6H11O5APP+O2=R311C6H11O7APPU     1.8E+0019 -2.500  0.0  !
R307C6H11O5APP+O2=R312C6H11O7APPU     1.8E+0019 -2.500  0.0  !
!Combinations to acids
R290C6H11O3AU+R3OOH=C6H11OKOOH+O2      3.07E11    0.    -
1.84E3  !
R290C6H11O3AU+R3OOH=C6H12O2B-1+O2+B1O  7.83E10    0.    -
1.84E3  !
!Combinations to alcoxy
2R290C6H11O3AU=2R35C6H11O2K+O2      1.81e11    0.00  -1391.0
!<Rosado-reyes2005>!
!Peracid decomposition
C6H11OKOOH=R2OH+R35C6H11O2K          4.00E+15    0.00  42900.0
!!C6H11OKO=CO2+R27C5H11              4.84E+10    1.11  15900.0
!!R35C6H11O2K+R3OOH=C6H12O2B-1+O2      3.07E11    0.    -
1.84E3
!!C6H11OKO+R1H=C6H12O2B-1            1.0E+14    0.0    0.0
!
R29C6H11OK+R3OOH=C6H11OKOOH          3.00E+13    0.0    0.0
!
R30C6H11OA+O2=R46C6H11O3AU          9.0E+0018 -2.500  0.0  ! ADO 35 CN
R31C6H11OA+O2=R48C6H11O3AU          1.7E+0019 -2.500  0.0  ! ADO 36 CN
R32C6H11OA+O2=R50C6H11O3AU          1.8E+0019 -2.500  0.0  ! ADO 37 CN
R33C6H11OA+O2=R51C6H11O3AU          1.8E+0019 -2.500  0.0  ! ADO 38 CN
R34C6H11OA+O2=R52C6H11O3AU          1.0E+0019 -2.500  0.0  ! ADO 39 CN
R36C6H11O2B+O2=R53C6H11O4UB          9.0E+0018 -2.500  0.0  ! ADO 40 CN
R37C6H11O2B+O2=R55C6H11O4UB          1.7E+0019 -2.500  0.0  ! ADO 41 CN
R38C6H11O2B+O2=R57C6H11O4UB          1.8E+0019 -2.500  0.0  ! ADO 42 CN
R39C6H11O2B+O2=R58C6H11O4UB          1.8E+0019 -2.500  0.0  ! ADO 43 CN
R40C6H11O2B+O2=R59C6H11O4UB          1.0E+0019 -2.500  0.0  ! ADO 44 CN

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R47C4H70A+O2=R79C4H703AU	9.0E+0018	-2.500	0.0	!	ADO 45	CN
R49C3H50A+O2=R86C3H503AU	9.0E+0018	-2.500	0.0	!	ADO 46	CN
R54C4H702B+O2=R106C4H704UB	9.0E+0018	-2.500	0.0	!	ADO 47	CN
R56C3H502B+O2=R111C3H504UB	9.0E+0018	-2.500	0.0	!	ADO 48	CN
R60C3H702P+O2=R124C3H704UP	1.7E+0019	-2.500	0.0	!	ADO 49	CN
R61C3H702P+O2=R125C3H704UP	9.0E+0018	-2.500	0.0	!	ADO 50	CN
R62C4H902P+O2=R126C4H904UP	1.8E+0019	-2.500	0.0	!	ADO 51	CN
R63C4H902P+O2=R127C4H904UP	1.7E+0019	-2.500	0.0	!	ADO 52	CN
R64C4H902P+O2=R128C4H904UP	9.0E+0018	-2.500	0.0	!	ADO 53	CN
!						
R65C5H1102P+O2=R129C5H1104UP	9.5E+0018	-2.500	0.0	!	ADO 54	CN
R66C5H1102P+O2=R130C5H1104UP	9.0E+0018	-2.500	0.0	!	ADO 55	CN
R67C5H1102P+O2=R132C5H1104UP	1.8E+0019	-2.500	0.0	!	ADO 56	CN
R68C5H1102P+O2=R133C5H1104UP	1.8E+0019	-2.500	0.0	!	ADO 57	CN
R69C5H1102P+O2=R134C5H1104UP	1.7E+0019	-2.500	0.0	!	ADO 58	CN
R70C5H1102P+O2=R135C5H1104UP	9.0E+0018	-2.500	0.0	!	ADO 59	CN
R71C5H1102P+O2=R136C5H1104UP	1.5E+0018	-2.500	0.0	!	ADO 60	CN
R72C5H1102P+O2=R137C5H1104UP	1.0E+0019	-2.500	0.0	!	ADO 61	CN
R73C5H1102P+O2=R138C5H1104UP	1.7E+0019	-2.500	0.0	!	ADO 62	CN
R74C5H1102P+O2=R139C5H1104UP	9.0E+0018	-2.500	0.0	!	ADO 63	CN
!						
!R65C5H1102P+O2=R129C5H1104UP	19.0E+0018	-2.500	0.0	!		
!R66C5H1102P+O2=R130C5H1104UP	18.0E+0018	-2.500	0.0	!		
!R67C5H1102P+O2=R132C5H1104UP	3.6E+0019	-2.500	0.0	!		
!R68C5H1102P+O2=R133C5H1104UP	3.6E+0019	-2.500	0.0	!		
!R69C5H1102P+O2=R134C5H1104UP	3.4E+0019	-2.500	0.0	!		
!R70C5H1102P+O2=R135C5H1104UP	18.0E+0018	-2.500	0.0	!		
!R71C5H1102P+O2=R136C5H1104UP	3.0E+0018	-2.500	0.0	!		
!R72C5H1102P+O2=R137C5H1104UP	2.0E+0019	-2.500	0.0	!		
!R73C5H1102P+O2=R138C5H1104UP	3.4E+0019	-2.500	0.0	!		
!R74C5H1102P+O2=R139C5H1104UP	18.0E+0018	-2.500	0.0	!		
!						
R75C6H1103AP+O2=R141C6H1105AUP	1.8E+0019	-2.500	0.0	!	ADO 64	CN
R76C6H1103AP+O2=R143C6H1105AUP	1.8E+0019	-2.500	0.0	!	ADO 65	CN
R77C6H1103AP+O2=R144C6H1105AUP	1.8E+0019	-2.500	0.0	!	ADO 66	CN
R78C6H1103AP+O2=R145C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 67	CN
R81C6H1103AP+O2=R149C6H1105AUP	1.5E+0018	-2.500	0.0	!	ADO 68	CN
R82C6H1103AP+O2=R150C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 69	CN
R83C6H1103AP+O2=R151C6H1105AUP	1.8E+0019	-2.500	0.0	!	ADO 70	CN
R84C6H1103AP+O2=R152C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 71	CN
R87C6H1103AP+O2=R155C6H1105AUP	9.5E+0018	-2.500	0.0	!	ADO 72	CN
R88C6H1103AP+O2=R156C6H1105AUP	9.0E+0018	-2.500	0.0	!	ADO 73	CN
R89C6H1103AP+O2=R158C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 74	CN
R90C6H1103AP+O2=R159C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 75	CN
R92C6H1103AP+O2=R160C6H1105AUP	3.0E+0018	-2.500	0.0	!	ADO 76	CN
R94C6H1103AP+O2=R161C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 77	CN
R95C6H1103AP+O2=R162C6H1105AUP	1.7E+0019	-2.500	0.0	!	ADO 78	CN
R96C6H1103AP+O2=R164C6H1105AUP	9.0E+0018	-2.500	0.0	!	ADO 79	CN
R98C6H1103AP+O2=R167C6H1105AUP	1.0E+0019	-2.500	0.0	!	ADO 80	CN
R99C6H1103AP+O2=R168C6H1105AUP	1.8E+0019	-2.500	0.0	!	ADO 81	CN
R100C6H1103AP+O2=R169C6H1105AUP	1.7E+0019	-2.500	0.0	!	ADO 82	CN
R101C6H1103AP+O2=R171C6H1105AUP	9.0E+0018	-2.500	0.0	!	ADO 83	CN
R102C6H1104PB+O2=R173C6H1106UPB	1.8E+0019	-2.500	0.0	!	ADO 84	CN
R103C6H1104PB+O2=R174C6H1106UPB	1.8E+0019	-2.500	0.0	!	ADO 85	CN
R104C6H1104PB+O2=R175C6H1106UPB	1.8E+0019	-2.500	0.0	!	ADO 86	CN
R105C6H1104PB+O2=R176C6H1106UPB	1.0E+0019	-2.500	0.0	!	ADO 87	CN
R107C6H1104PB+O2=R179C6H1106UPB	1.5E+0018	-2.500	0.0	!	ADO 88	CN
R108C6H1104PB+O2=R180C6H1106UPB	1.0E+0019	-2.500	0.0	!	ADO 89	CN



R109C6H11O4PB+O2=R181C6H11O6UPB	1.8E+0019	-2.500	0.0	!	ADO 90	CN
R110C6H11O4PB+O2=R182C6H11O6UPB	1.0E+0019	-2.500	0.0	!	ADO 91	CN
R112C6H11O4PB+O2=R184C6H11O6UPB	9.5E+0018	-2.500	0.0	!	ADO 92	CN
R113C6H11O4PB+O2=R185C6H11O6UPB	9.0E+0018	-2.500	0.0	!	ADO 93	CN
R114C6H11O4PB+O2=R187C6H11O6UPB	1.0E+0019	-2.500	0.0	!	ADO 94	CN
R115C6H11O4PB+O2=R188C6H11O6UPB	1.0E+0019	-2.500	0.0	!	ADO 95	CN
R116C6H11O4PB+O2=R189C6H11O6UPB	2.5E+0018	-2.500	0.0	!	ADO 96	CN
R117C6H11O4PB+O2=R190C6H11O6UPB	1.0E+0019	-2.500	0.0	!	ADO 97	CN
R118C6H11O4PB+O2=R191C6H11O6UPB	1.7E+0019	-2.500	0.0	!	ADO 98	CN
R119C6H11O4PB+O2=R193C6H11O6UPB	9.0E+0018	-2.500	0.0	!	ADO 99	CN
R120C6H11O4PB+O2=R195C6H11O6UPB	1.0E+0019	-2.500	0.0	!	ADO 100	CN
R121C6H11O4PB+O2=R196C6H11O6UPB	1.8E+0019	-2.500	0.0	!	ADO 101	CN
R122C6H11O4PB+O2=R197C6H11O6UPB	1.7E+0019	-2.500	0.0	!	ADO 102	CN
R123C6H11O4PB+O2=R199C6H11O6UPB	9.0E+0018	-2.500	0.0	!	ADO 103	CN
R131C3H7O2P+O2=R201C3H7O4UP	1.0E+0019	-2.500	0.0	!	ADO 104	CN
R140C3H7O2P+O2=R202C3H7O4UP	1.5E+0018	-2.500	0.0	!	ADO 105	CN
R146C4H7O3AP+O2=R204C4H7O5AUP	1.8E+0019	-2.500	0.0	!	ADO 106	CN
R147C4H7O3AP+O2=R205C4H7O5AUP	1.0E+0019	-2.500	0.0	!	ADO 107	CN
R153C3H5O3AP+O2=R206C3H5O5AUP	1.0E+0019	-2.500	0.0	!	ADO 108	CN
R157C4H7O3AP+O2=R207C4H7O5AUP	1.0E+0019	-2.500	0.0	!	ADO 109	CN
R163C3H5O3AP+O2=R208C3H5O5AUP	1.0E+0019	-2.500	0.0	!	ADO 110	CN
R165C4H7O3AP+O2=R209C4H7O5AUP	1.5E+0018	-2.500	0.0	!	ADO 111	CN
R166C5H11O2P+O2=R212C5H11O4UP	1.0E+0019	-2.500	0.0	!	ADO 112	CN
R170C3H5O3AP+O2=R213C3H5O5AUP	1.5E+0018	-2.500	0.0	!	ADO 113	CN
R172C4H7O3AP+O2=R215C4H7O5AUP	9.0E+0018	-2.500	0.0	!	ADO 114	CN
R177C4H7O4PB+O2=R218C4H7O6UPB	1.8E+0019	-2.500	0.0	!	ADO 115	CN
R178C4H7O4PB+O2=R219C4H7O6UPB	1.0E+0019	-2.500	0.0	!	ADO 116	CN
R183C3H5O4PB+O2=R220C3H5O6UPB	1.0E+0019	-2.500	0.0	!	ADO 117	CN
R186C4H7O4PB+O2=R221C4H7O6UPB	1.0E+0019	-2.500	0.0	!	ADO 118	CN
R192C3H5O4PB+O2=R222C3H5O6UPB	1.0E+0019	-2.500	0.0	!	ADO 119	CN
R194C4H7O4PB+O2=R223C4H7O6UPB	1.5E+0018	-2.500	0.0	!	ADO 120	CN
R198C3H5O4PB+O2=R225C3H5O6UPB	1.5E+0018	-2.500	0.0	!	ADO 121	CN
R200C4H7O4PB+O2=R227C4H7O6UPB	9.0E+0018	-2.500	0.0	!	ADO 122	CN
R229C3H7+O2=R203C3H7O2U	1.6E+0019	-2.500	0.0	!	ADO 123	CN
R230C4H7O3AP+O2=R241C4H7O5AUP	3.0E+0018	-2.500	0.0	!	ADO 124	CN
R231C4H7O3AP+O2=R210C4H7O3AU	1.7E+0019	-2.500	0.0	!	ADO 125	CN
R233C3H5O3AP+O2=R214C3H5O3AU	9.5E+0018	-2.500	0.0	!	ADO 126	CN
R234C4H7O3AP+O2=R242C4H7O5AUP	9.5E+0018	-2.500	0.0	!	ADO 127	CN
R235C4H7O3AP+O2=R216C4H7O3AU	1.0E+0019	-2.500	0.0	!	ADO 128	CN
R236C4H7O4PB+O2=R243C4H7O6UPB	2.5E+0018	-2.500	0.0	!	ADO 129	CN
R237C4H7O2B+O2=R224C4H7O4UB	1.7E+0019	-2.500	0.0	!	ADO 130	CN
R238C3H5O2B+O2=R226C3H5O4UB	9.0E+0018	-2.500	0.0	!	ADO 131	CN
R239C4H7O4PB+O2=R244C4H7O6UPB	9.5E+0018	-2.500	0.0	!	ADO 132	CN
R240C4H7O2B+O2=R228C4H7O4UB	1.0E+0019	-2.500	0.0	!	ADO 133	CN

! isomerisations :

R27C5H11=R28C5H11	5.7E+0008	1.000	17300.0	!	IS 134	KB
R30C6H11OA=R33C6H11OA	5.7E+0008	1.000	17300.0	!	IS 135	KB
R30C6H11OA=R34C6H11OA	9.9E+0007	1.000	12000.0	!	IS 136	KB
R31C6H11OA=R34C6H11OA	5.7E+0008	1.000	17300.0	!	IS 137	KB

!

!Olive: Missing Isomerizations

R30C6H11OA=R29C6H11OK	8.48E+0006	1.000	8400.0	!	Dn=5,
rpd=1, Ea=11-9+6.4					
R31C6H11OA=R29C6H11OK	4.93E+0007	1.000	3000.0	!	Dn=4,
rpd=1, Ea=11-9+1					
R32C6H11OA=R29C6H11OK	2.87E+0008	1.000	8300.0	!	Dn=3,
rpd=1, Ea=11-9+6.3					

R33C6H110A=R29C6H110K	1.67E+0009	1.000	28000.0	!Dn=2,
rpd=1, Ea=11-9+26				
R290C6H1103AU=R291C6H1103AP	5.74E+0008	1.000	25500.0	
!Dn=3, rpd=2, Ea=17+8.5				
R290C6H1103AU=R292C6H1103AP	9.87E+0007	1.000	22000.0	
!Dn=4, rpd=2, Ea=17+5				
R290C6H1103AU=R293C6H1103AP	1.70E+0007	1.000	21000.0	
!Dn=5, rpd=2, Ea=17+4				
!C6H110KOO=C6H10OKOOH3	5.74E+0008	1.000	25500.0	!
!C6H110KOO=C6H10OKOOH4	4.26E+0006	1.37	17900.0	!Villano
!C6H110KOO=C6H10OKOOH5	1.76E+0006	1.20	16900.0	!Villano
R300C6H1105APU=R305C6H1105APP	5.74E+0008	1.000	25500.0	
!Dn=3, rpd=2, Ea=17+8.5				
R301C6H1105APU=R306C6H1105APP	5.74E+0008	1.000	25500.0	
!Dn=3, rpd=2, Ea=17+8.5				
R302C6H1105APU=R307C6H1105APP	5.74E+0008	1.000	25500.0	
!Dn=3, rpd=2, Ea=17+8.5				
R310C6H1107APPU=R20H+C6H8OK(OOH) 20	4.93E+0007	1.000	23500.0	!Dn=3,
rpd=1, Ea=17-2+8.5				
R311C6H1107APPU=R20H+C6H8OK(OOH) 20	4.93E+0007	1.000	23500.0	!Dn=3,
rpd=1, Ea=17-2+8.5				
R312C6H1107APPU=R20H+C6H8OK(OOH) 20	4.93E+0007	1.000	23500.0	!Dn=3,
rpd=1, Ea=17-2+8.5				
C6H8OK(OOH) 20=>R20H+CO2+CH2COZ+C3H6Z+R3OOH	1.5E+0016	0.000	43000.0	!
!C6H8OK(OOH) 20=>2R20H+CO2+CH2COZ+C2H6CO	1.5E+0016	0.000	43000.0	!
!				
R36C6H1102B=R39C6H1102B	5.7E+0008	1.000	17300.0	! IS 138 KB
R36C6H1102B=R40C6H1102B	9.9E+0007	1.000	12000.0	! IS 139 KB
R37C6H1102B=R40C6H1102B	5.7E+0008	1.000	17300.0	! IS 140 KB
R41C3H7O2U=R60C3H7O2P	3.3E+0009	1.000	32500.0	! IS 141 KB
R41C3H7O2U=R61C3H7O2P	8.6E+0008	1.000	28500.0	! IS 142 KB
R42C4H9O2U=R62C4H9O2P	3.3E+0009	1.000	32500.0	! IS 143 KB
R42C4H9O2U=R63C4H9O2P	5.7E+0008	1.000	25500.0	! IS 144 KB
R42C4H9O2U=R64C4H9O2P	1.5E+0008	1.000	25000.0	! IS 145 KB
R43C5H1102U=R65C5H1102P	6.7E+0009	1.000	32500.0	! IS 146 KB
R43C5H1102U=R66C5H1102P	1.7E+0009	1.000	28500.0	! IS 147 KB
R44C5H1102U=R67C5H1102P	3.3E+0009	1.000	32500.0	! IS 148 KB
R44C5H1102U=R68C5H1102P	5.7E+0008	1.000	25500.0	! IS 149 KB
R44C5H1102U=R69C5H1102P	9.9E+0007	1.000	22000.0	! IS 150 KB
R44C5H1102U=R70C5H1102P	2.5E+0007	1.000	24000.0	! IS 151 KB
R45C5H1102U=R71C5H1102P	5.0E+0009	1.000	35500.0	! IS 152 KB
R45C5H1102U=R72C5H1102P	3.3E+0009	1.000	32500.0	! IS 153 KB
R45C5H1102U=R73C5H1102P	5.7E+0008	1.000	25500.0	! IS 154 KB
R45C5H1102U=R74C5H1102P	1.5E+0008	1.000	25000.0	! IS 155 KB
R46C6H1103AU=R75C6H1103AP	3.3E+0009	1.000	32500.0	! IS 156 KB
R46C6H1103AU=R76C6H1103AP	5.7E+0008	1.000	25500.0	! IS 157 KB
R46C6H1103AU=R77C6H1103AP	9.9E+0007	1.000	22000.0	! IS 158 KB
R46C6H1103AU=R78C6H1103AP	1.7E+0007	1.000	21000.0	! IS 159 KB
R47C4H7OA=R80C4H7OK	2.9E+0008	1.000	13300.0	! IS 160 KB
R48C6H1103AU=R81C6H1103AP	5.0E+0009	1.000	35500.0	! IS 161 KB
R48C6H1103AU=R82C6H1103AP	3.3E+0009	1.000	32500.0	! IS 162 KB
R48C6H1103AU=R83C6H1103AP	5.7E+0008	1.000	25500.0	! IS 163 KB
R48C6H1103AU=R84C6H1103AP	9.9E+0007	1.000	22000.0	! IS 164 KB
R48C6H1103AU=R85C6H1103KP	8.5E+0006	1.000	16000.0	! IS 165 KB
R50C6H1103AU=R87C6H1103AP	3.3E+0009	1.000	32500.0	! IS 166 KB
R50C6H1103AU=R88C6H1103AP	8.6E+0008	1.000	28500.0	! IS 167 KB
R50C6H1103AU=R89C6H1103AP	3.3E+0009	1.000	32500.0	! IS 168 KB
R50C6H1103AU=R90C6H1103AP	5.7E+0008	1.000	25500.0	! IS 169 KB

R50C6H1103AU=R91C6H1103KP	4.9E+0007	1.000	17000.0	! IS 170 KB
R51C6H1103AU=R92C6H1103AP	3.3E+0009	1.000	32500.0	! IS 171 KB
R51C6H1103AU=R93C6H1103KP	2.9E+0008	1.000	20500.0	! IS 172 KB
R51C6H1103AU=R94C6H1103AP	3.3E+0009	1.000	32500.0	! IS 173 KB
R51C6H1103AU=R95C6H1103AP	5.7E+0008	1.000	25500.0	! IS 174 KB
R51C6H1103AU=R96C6H1103AP	1.5E+0008	1.000	25000.0	! IS 175 KB
R52C6H1103AU=R97C6H1103KP	1.7E+0009	1.000	27500.0	! IS 176 KB
R52C6H1103AU=R98C6H1103AP	3.3E+0009	1.000	32500.0	! IS 177 KB
R52C6H1103AU=R99C6H1103AP	5.7E+0008	1.000	25500.0	! IS 178 KB
R52C6H1103AU=R100C6H1103AP	9.9E+0007	1.000	22000.0	! IS 179 KB
R52C6H1103AU=R101C6H1103AP	2.5E+0007	1.000	24000.0	! IS 180 KB
R53C6H1104UB=R102C6H1104PB	3.3E+0009	1.000	32500.0	! IS 181 KB
R53C6H1104UB=R103C6H1104PB	5.7E+0008	1.000	25500.0	! IS 182 KB
R53C6H1104UB=R104C6H1104PB	9.9E+0007	1.000	22000.0	! IS 183 KB
R53C6H1104UB=R105C6H1104PB	1.7E+0007	1.000	21000.0	! IS 184 KB
R55C6H1104UB=R107C6H1104PB	5.0E+0009	1.000	35500.0	! IS 185 KB
R55C6H1104UB=R108C6H1104PB	3.3E+0009	1.000	32500.0	! IS 186 KB
R55C6H1104UB=R109C6H1104PB	5.7E+0008	1.000	25500.0	! IS 187 KB
R55C6H1104UB=R110C6H1104PB	9.9E+0007	1.000	22000.0	! IS 188 KB
R57C6H1104UB=R112C6H1104PB	3.3E+0009	1.000	32500.0	! IS 189 KB
R57C6H1104UB=R113C6H1104PB	8.6E+0008	1.000	28500.0	! IS 190 KB
R57C6H1104UB=R114C6H1104PB	3.3E+0009	1.000	32500.0	! IS 191 KB
R57C6H1104UB=R115C6H1104PB	5.7E+0008	1.000	25500.0	! IS 192 KB
R58C6H1104UB=R116C6H1104PB	3.3E+0009	1.000	32500.0	! IS 193 KB
R58C6H1104UB=R117C6H1104PB	3.3E+0009	1.000	32500.0	! IS 194 KB
R58C6H1104UB=R118C6H1104PB	5.7E+0008	1.000	25500.0	! IS 195 KB
R58C6H1104UB=R119C6H1104PB	1.5E+0008	1.000	25000.0	! IS 196 KB
R59C6H1104UB=R120C6H1104PB	3.3E+0009	1.000	32500.0	! IS 197 KB
R59C6H1104UB=R121C6H1104PB	5.7E+0008	1.000	25500.0	! IS 198 KB
R59C6H1104UB=R122C6H1104PB	9.9E+0007	1.000	22000.0	! IS 199 KB
R59C6H1104UB=R123C6H1104PB	2.5E+0007	1.000	24000.0	! IS 200 KB
R65C5H1102P=R66C5H1102P	8.6E+0008	1.000	19800.0	! IS 201 KB
R67C5H1102P=R70C5H1102P	8.6E+0008	1.000	19800.0	! IS 202 KB
R71C5H1102P=R73C5H1102P	5.7E+0008	1.000	17300.0	! IS 203 KB
R71C5H1102P=R74C5H1102P	1.5E+0008	1.000	14500.0	! IS 204 KB
R75C6H1103AP=R78C6H1103AP	5.7E+0008	1.000	17300.0	! IS 205 KB
R75C6H1103AP=R142C6H1103KP	4.9E+0007	1.000	8000.0	! IS 206 KB
R76C6H1103AP=R142C6H1103KP	2.9E+0008	1.000	13300.0	! IS 207 KB
R79C4H703AU=R146C4H703AP	3.3E+0009	1.000	32500.0	! IS 208 KB
R79C4H703AU=R147C4H703AP	5.7E+0008	1.000	25500.0	! IS 209 KB
R79C4H703AU=R148C4H703KP	4.9E+0007	1.000	17000.0	! IS 210 KB
R81C6H1103AP=R83C6H1103AP	5.7E+0008	1.000	17300.0	! IS 211 KB
R81C6H1103AP=R84C6H1103AP	9.9E+0007	1.000	12000.0	! IS 212 KB
R81C6H1103AP=R85C6H1103KP	8.5E+0006	1.000	13400.0	! IS 213 KB
R82C6H1103AP=R85C6H1103KP	2.9E+0008	1.000	13300.0	! IS 214 KB
R86C3H503AU=R153C3H503AP	3.3E+0009	1.000	32500.0	! IS 215 KB
R86C3H503AU=R154C3H503KP	2.9E+0008	1.000	20500.0	! IS 216 KB
R87C6H1103AP=R90C6H1103AP	5.7E+0008	1.000	17300.0	! IS 217 KB
R87C6H1103AP=R91C6H1103KP	4.9E+0007	1.000	8000.0	! IS 218 KB
R88C6H1103AP=R89C6H1103AP	5.7E+0008	1.000	17300.0	! IS 219 KB
R88C6H1103AP=R90C6H1103AP	9.9E+0007	1.000	12000.0	! IS 220 KB
R88C6H1103AP=R91C6H1103KP	8.5E+0006	1.000	13400.0	! IS 221 KB
R92C6H1103AP=R95C6H1103AP	5.7E+0008	1.000	17300.0	! IS 222 KB
R92C6H1103AP=R96C6H1103AP	1.5E+0008	1.000	14500.0	! IS 223 KB
R98C6H1103AP=R101C6H1103AP	8.6E+0008	1.000	19800.0	! IS 224 KB
R102C6H1104PB=R105C6H1104PB	5.7E+0008	1.000	17300.0	! IS 225 KB
R106C4H704UB=R177C4H704PB	3.3E+0009	1.000	32500.0	! IS 226 KB
R106C4H704UB=R178C4H704PB	5.7E+0008	1.000	25500.0	! IS 227 KB

R107C6H11O4PB=R109C6H11O4PB	5.7E+0008	1.000	17300.0	!	IS 228 KB
R107C6H11O4PB=R110C6H11O4PB	9.9E+0007	1.000	12000.0	!	IS 229 KB
R111C3H5O4UB=R183C3H5O4PB	3.3E+0009	1.000	32500.0	!	IS 230 KB
R112C6H11O4PB=R115C6H11O4PB	5.7E+0008	1.000	17300.0	!	IS 231 KB
R113C6H11O4PB=R114C6H11O4PB	5.7E+0008	1.000	17300.0	!	IS 232 KB
R113C6H11O4PB=R115C6H11O4PB	9.9E+0007	1.000	12000.0	!	IS 233 KB
R116C6H11O4PB=R118C6H11O4PB	5.7E+0008	1.000	17300.0	!	IS 234 KB
R116C6H11O4PB=R119C6H11O4PB	1.5E+0008	1.000	14500.0	!	IS 235 KB
R120C6H11O4PB=R123C6H11O4PB	8.6E+0008	1.000	19800.0	!	IS 236 KB
R203C3H7O2U=R140C3H7O2P	1.0E+0010	1.000	33500.0	!	IS 237 KB
R210C4H7O3AU=R165C4H7O3AP	5.0E+0009	1.000	33500.0	!	IS 238 KB
R165C4H7O3AP=R211C4H7O3KP	2.9E+0008	1.000	13300.0	!	IS 239 KB
R214C3H5O3AU=R170C3H5O3AP	5.0E+0009	1.000	33500.0	!	IS 240 KB
R216C4H7O3AU=R172C4H7O3AP	8.6E+0008	1.000	26500.0	!	IS 241 KB
R172C4H7O3AP=R217C4H7O3KP	2.9E+0008	1.000	13300.0	!	IS 242 KB
R224C4H7O4UB=R194C4H7O4PB	5.0E+0009	1.000	33500.0	!	IS 243 KB
R226C3H5O4UB=R198C3H5O4PB	5.0E+0009	1.000	33500.0	!	IS 244 KB
R228C4H7O4UB=R200C4H7O4PB	8.6E+0008	1.000	26500.0	!	IS 245 KB
R210C4H7O3AU=R230C4H7O3AP	3.3E+0009	1.000	32500.0	!	IS 246 KB
R210C4H7O3AU=R211C4H7O3KP	2.9E+0008	1.000	20500.0	!	IS 247 KB
R214C3H5O3AU=R232C3H5O3KP	1.7E+0009	1.000	27500.0	!	IS 248 KB
R216C4H7O3AU=R217C4H7O3KP	1.7E+0009	1.000	27500.0	!	IS 249 KB
R216C4H7O3AU=R234C4H7O3AP	3.3E+0009	1.000	32500.0	!	IS 250 KB
R224C4H7O4UB=R236C4H7O4PB	3.3E+0009	1.000	32500.0	!	IS 251 KB
R228C4H7O4UB=R239C4H7O4PB	3.3E+0009	1.000	32500.0	!	IS 252 KB

! Decomposition of OOQOOH into branching agents:

R64C4H9O2P=>R2OH+C4H8OA	5.7E+0008	1.000	15300.0	!	253 KB
R69C5H11O2P=>R2OH+C5H10OA	5.7E+0008	1.000	15300.0	!	254 KB
R70C5H11O2P=>R2OH+C5H10OA	9.9E+0007	1.000	10000.0	!	255 KB
R74C5H11O2P=>R2OH+C5H10OK	2.9E+0008	1.000	13300.0	!	256 KB
R77C6H11O3AP=>R2OH+C6H10O2A	5.7E+0008	1.000	15300.0	!	257 KB
R78C6H11O3AP=>R2OH+C6H10O2A	9.9E+0007	1.000	10000.0	!	258 KB
R84C6H11O3AP=>R2OH+C6H10O2KA	2.9E+0008	1.000	13300.0	!	259 KB
R96C6H11O3AP=>R2OH+C6H10O2KA	2.9E+0008	1.000	13300.0	!	260 KB
R100C6H11O3AP=>R2OH+C6H10O2KA	2.9E+0008	1.000	13300.0	!	261 KB
R101C6H11O3AP=>R2OH+C6H10O2KA	4.9E+0007	1.000	8000.0	!	262 KB
R104C6H11O4PB=>R2OH+C6H10O3AB	5.7E+0008	1.000	15300.0	!	263 KB
R105C6H11O4PB=>R2OH+C6H10O3AB	9.9E+0007	1.000	10000.0	!	264 KB
R110C6H11O4PB=>R2OH+C6H10O3KB	2.9E+0008	1.000	13300.0	!	265 KB
R119C6H11O4PB=>R2OH+C6H10O3KB	2.9E+0008	1.000	13300.0	!	266 KB
R122C6H11O4PB=>R2OH+C6H10O3KB	2.9E+0008	1.000	13300.0	!	267 KB
R123C6H11O4PB=>R2OH+C6H10O3KB	4.9E+0007	1.000	8000.0	!	268 KB
R124C3H7O4UP=>R2OH+C3H6O3KP	5.0E+0009	1.000	35500.0	!	269 KB
DUPLICATE					
R124C3H7O4UP=>R2OH+C3H6O3KP	3.3E+0009	1.000	30500.0	!	270 KB
DUPLICATE					
R125C3H7O4UP=>R2OH+C3H6O3KP	3.3E+0009	1.000	32500.0	!	271 KB
DUPLICATE					
R125C3H7O4UP=>R2OH+C3H6O3KP	5.7E+0008	1.000	23500.0	!	272 KB
DUPLICATE					
R126C4H9O4UP=>R2OH+C4H8O3KP	3.3E+0009	1.000	30500.0	!	273 KB
DUPLICATE					
R126C4H9O4UP=>R2OH+C4H8O3KP	3.3E+0009	1.000	32500.0	!	274 KB
DUPLICATE					
R126C4H9O4UP=>R2OH+C4H8O3KP	8.6E+0008	1.000	28500.0	!	275 KB
DUPLICATE					
R127C4H9O4UP=>R2OH+C4H8O3KP	5.0E+0009	1.000	35500.0	!	276 KB

DUPLICATE						
R127C4H9O4UP=>R2OH+C4H8O3KP	3.3E+0009	1.000	32500.0	!	277	KB
DUPLICATE						
R127C4H9O4UP=>R2OH+C4H8O3KP	5.7E+0008	1.000	23500.0	!	278	KB
DUPLICATE						
R128C4H9O4UP=>R2OH+C4H8O3KP	5.7E+0008	1.000	32500.0	!	279	KB
DUPLICATE						
R128C4H9O4UP=>R2OH+C4H8O3KP	5.7E+0008	1.000	25500.0	!	280	KB
DUPLICATE						
R128C4H9O4UP=>R2OH+C4H8O3KP	9.9E+0007	1.000	20000.0	!	281	KB
DUPLICATE						
R129C5H11O4UP=>R2OH+C5H10O3KP	5.0E+0009	1.000	35500.0	!	282	KB
DUPLICATE						
R129C5H11O4UP=>R2OH+C5H10O3KP	1.7E+0009	1.000	27500.0	!	283	KB
DUPLICATE						
R129C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	284	KB
DUPLICATE						
R129C5H11O4UP=>R2OH+C5H10O3KP	1.5E+0008	1.000	25000.0	!	285	KB
DUPLICATE						
R130C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	286	KB
DUPLICATE						
R130C5H11O4UP=>R2OH+C5H10O3KP	2.9E+0008	1.000	20500.0	!	287	KB
DUPLICATE						
R130C5H11O4UP=>R2OH+C5H10O3KP	9.9E+0007	1.000	22000.0	!	288	KB
DUPLICATE						
R130C5H11O4UP=>R2OH+C5H10O3KP	2.5E+0007	1.000	24000.0	!	289	KB
DUPLICATE						
R132C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	30500.0	!	290	KB
DUPLICATE						
R132C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	291	KB
DUPLICATE						
R132C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	292	KB
DUPLICATE						
R132C5H11O4UP=>R2OH+C5H10O3KP	1.5E+0008	1.000	25000.0	!	293	KB
DUPLICATE						
R133C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	294	KB
DUPLICATE						
R133C5H11O4UP=>R2OH+C5H10O3KP	8.6E+0008	1.000	28500.0	!	295	KB
DUPLICATE						
R133C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	296	KB
DUPLICATE						
R133C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	23500.0	!	297	KB
DUPLICATE						
R134C5H11O4UP=>R2OH+C5H10O3KP	5.0E+0009	1.000	35500.0	!	298	KB
DUPLICATE						
R134C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	299	KB
DUPLICATE						
R134C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	300	KB
DUPLICATE						
R134C5H11O4UP=>R2OH+C5H10O3KP	9.9E+0007	1.000	20000.0	!	301	KB
DUPLICATE						
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DUPLICATE						
R135C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	303	KB
DUPLICATE						
R135C5H11O4UP=>R2OH+C5H10O3KP	9.9E+0007	1.000	22000.0	!	304	KB
DUPLICATE						
R135C5H11O4UP=>R2OH+C5H10O3KP	1.7E+0007	1.000	19000.0	!	305	KB

DUPLICATE						
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DUPLICATE						
R136C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	307	KB
DUPLICATE						
R136C5H11O4UP=>R2OH+C5H10O3KP	9.9E+0007	1.000	22000.0	!	308	KB
DUPLICATE						
R136C5H11O4UP=>R2OH+C5H10O3KP	2.5E+0007	1.000	24000.0	!	309	KB
DUPLICATE						
R137C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	310	KB
DUPLICATE						
R137C5H11O4UP=>R2OH+C5H10O3KP	8.6E+0008	1.000	28500.0	!	311	KB
DUPLICATE						
R137C5H11O4UP=>R2OH+C5H10O3KP	1.7E+0009	1.000	27500.0	!	312	KB
DUPLICATE						
R137C5H11O4UP=>R2OH+C5H10O3KP	8.6E+0008	1.000	28500.0	!	313	KB
DUPLICATE						
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DUPLICATE						
R138C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	315	KB
DUPLICATE						
R138C5H11O4UP=>R2OH+C5H10O3KP	2.9E+0008	1.000	20500.0	!	316	KB
DUPLICATE						
R138C5H11O4UP=>R2OH+C5H10O3KP	1.5E+0008	1.000	25000.0	!	317	KB
DUPLICATE						
R139C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	318	KB
DUPLICATE						
R139C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	319	KB
DUPLICATE						
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DUPLICATE						
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DUPLICATE						
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DUPLICATE						
R141C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	323	KB
DUPLICATE						
R141C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	324	KB
DUPLICATE						
R141C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	325	KB
DUPLICATE						
R141C6H11O5AUP=>R2OH+C6H10O4KAP	8.5E+0006	1.000	16000.0	!	326	KB
DUPLICATE						
R143C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	327	KB
DUPLICATE						
R143C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	23500.0	!	328	KB
DUPLICATE						
R143C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	329	KB
DUPLICATE						
R143C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	330	KB
DUPLICATE						
R143C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	331	KB
DUPLICATE						
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DUPLICATE						
R144C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	333	KB
DUPLICATE						
R144C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	334	KB

DUPLICATE					
R144C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	335 KB
DUPLICATE					
R144C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	20000.0	!	336 KB
DUPLICATE					
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DUPLICATE					
R145C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	338 KB
DUPLICATE					
R145C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	339 KB
DUPLICATE					
R145C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	340 KB
DUPLICATE					
R145C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0007	1.000	19000.0	!	341 KB
DUPLICATE					
R149C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	342 KB
DUPLICATE					
R149C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	343 KB
DUPLICATE					
R149C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	344 KB
DUPLICATE					
R149C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0007	1.000	21000.0	!	345 KB
DUPLICATE					
R150C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	346 KB
DUPLICATE					
R150C6H11O5AUP=>R2OH+C6H10O4KAP	8.6E+0008	1.000	28500.0	!	347 KB
DUPLICATE					
R150C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	348 KB
DUPLICATE					
R150C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	349 KB
DUPLICATE					
R150C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	350 KB
DUPLICATE					
R151C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	351 KB
DUPLICATE					
R151C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	352 KB
DUPLICATE					
R151C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	353 KB
DUPLICATE					
R151C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	354 KB
DUPLICATE					
R151C6H11O5AUP=>R2OH+C6H10O4KAP	1.5E+0008	1.000	25000.0	!	355 KB
DUPLICATE					
R152C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	356 KB
DUPLICATE					
R152C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	357 KB
DUPLICATE					
R152C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	358 KB
DUPLICATE					
R152C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	359 KB
DUPLICATE					
R152C6H11O5AUP=>R2OH+C6H10O4KAP	2.5E+0007	1.000	24000.0	!	360 KB
DUPLICATE					
R155C6H11O5AUP=>R2OH+C6H10O4KAP	5.0E+0009	1.000	35500.0	!	361 KB
DUPLICATE					
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DUPLICATE					
R155C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	363 KB

DUPLICATE					
R155C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	364 KB
DUPLICATE					
R155C6H11O5AUP=>R2OH+C6H10O4KAP	8.5E+0006	1.000	16000.0	!	365 KB
DUPLICATE					
R156C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	366 KB
DUPLICATE					
R156C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	367 KB
DUPLICATE					
R156C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	368 KB
DUPLICATE					
R156C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0007	1.000	21000.0	!	369 KB
DUPLICATE					
R158C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	370 KB
DUPLICATE					
R158C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	371 KB
DUPLICATE					
R158C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	372 KB
DUPLICATE					
R158C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	373 KB
DUPLICATE					
R158C6H11O5AUP=>R2OH+C6H10O4KAP	1.5E+0008	1.000	25000.0	!	374 KB
DUPLICATE					
R159C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	375 KB
DUPLICATE					
R159C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	376 KB
DUPLICATE					
R159C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	377 KB
DUPLICATE					
R159C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	378 KB
DUPLICATE					
R159C6H11O5AUP=>R2OH+C6H10O4KAP	2.5E+0007	1.000	24000.0	!	379 KB
DUPLICATE					
R160C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	380 KB
DUPLICATE					
R160C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	381 KB
DUPLICATE					
R160C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	382 KB
DUPLICATE					
R160C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	383 KB
DUPLICATE					
R160C6H11O5AUP=>R2OH+C6H10O4KAP	2.5E+0007	1.000	24000.0	!	384 KB
DUPLICATE					
R161C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	385 KB
DUPLICATE					
R161C6H11O5AUP=>R2OH+C6H10O4KAP	8.6E+0008	1.000	28500.0	!	386 KB
DUPLICATE					
R161C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	387 KB
DUPLICATE					
R161C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	388 KB
DUPLICATE					
R161C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	389 KB
DUPLICATE					
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DUPLICATE					
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DUPLICATE					
R162C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	392 KB



DUPLICATE					
R162C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	393 KB
DUPLICATE					
R162C6H11O5AUP=>R2OH+C6H10O4KAP	8.5E+0006	1.000	16000.0	!	394 KB
DUPLICATE					
R164C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	395 KB
DUPLICATE					
R164C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	396 KB
DUPLICATE					
R164C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	397 KB
DUPLICATE					
R164C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0007	1.000	21000.0	!	398 KB
DUPLICATE					
R167C6H11O5AUP=>R2OH+C6H10O4KAP	1.7E+0009	1.000	27500.0	!	399 KB
DUPLICATE					
R167C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	400 KB
DUPLICATE					
R167C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	401 KB
DUPLICATE					
R167C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	402 KB
DUPLICATE					
R167C6H11O5AUP=>R2OH+C6H10O4KAP	1.5E+0008	1.000	25000.0	!	403 KB
DUPLICATE					
R168C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	404 KB
DUPLICATE					
R168C6H11O5AUP=>R2OH+C6H10O4KAP	8.6E+0008	1.000	28500.0	!	405 KB
DUPLICATE					
R168C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	406 KB
DUPLICATE					
R168C6H11O5AUP=>R2OH+C6H10O4KAP	2.9E+0008	1.000	20500.0	!	407 KB
DUPLICATE					
R168C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	408 KB
DUPLICATE					
R169C6H11O5AUP=>R2OH+C6H10O4KAP	5.0E+0009	1.000	35500.0	!	409 KB
DUPLICATE					
R169C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	410 KB
DUPLICATE					
R169C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	411 KB
DUPLICATE					
R169C6H11O5AUP=>R2OH+C6H10O4KAP	4.9E+0007	1.000	17000.0	!	412 KB
DUPLICATE					
R169C6H11O5AUP=>R2OH+C6H10O4KAP	8.5E+0006	1.000	16000.0	!	413 KB
DUPLICATE					
R171C6H11O5AUP=>R2OH+C6H10O4KAP	3.3E+0009	1.000	32500.0	!	414 KB
DUPLICATE					
R171C6H11O5AUP=>R2OH+C6H10O4KAP	5.7E+0008	1.000	25500.0	!	415 KB
DUPLICATE					
R171C6H11O5AUP=>R2OH+C6H10O4KAP	9.9E+0007	1.000	22000.0	!	416 KB
DUPLICATE					
R171C6H11O5AUP=>R2OH+C6H10O4KAP	8.5E+0006	1.000	16000.0	!	417 KB
DUPLICATE					
R173C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	30500.0	!	418 KB
DUPLICATE					
R173C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	419 KB
DUPLICATE					
R173C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	420 KB
DUPLICATE					
R173C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	421 KB

DUPLICATE					
R174C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	422 KB
DUPLICATE					
R174C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	23500.0	!	423 KB
DUPLICATE					
R174C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	424 KB
DUPLICATE					
R174C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	425 KB
DUPLICATE					
R175C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	426 KB
DUPLICATE					
R175C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	427 KB
DUPLICATE					
R175C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	428 KB
DUPLICATE					
R175C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	20000.0	!	429 KB
DUPLICATE					
R176C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	430 KB
DUPLICATE					
R176C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	431 KB
DUPLICATE					
R176C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	432 KB
DUPLICATE					
R176C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0007	1.000	19000.0	!	433 KB
DUPLICATE					
R179C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	434 KB
DUPLICATE					
R179C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	435 KB
DUPLICATE					
R179C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	436 KB
DUPLICATE					
R179C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0007	1.000	21000.0	!	437 KB
DUPLICATE					
R180C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	438 KB
DUPLICATE					
R180C6H11O6UPB=>R2OH+C6H10O5KPB	8.6E+0008	1.000	28500.0	!	439 KB
DUPLICATE					
R180C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	440 KB
DUPLICATE					
R180C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	441 KB
DUPLICATE					
R181C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	442 KB
DUPLICATE					
R181C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	443 KB
DUPLICATE					
R181C6H11O6UPB=>R2OH+C6H10O5KPB	2.9E+0008	1.000	20500.0	!	444 KB
DUPLICATE					
R181C6H11O6UPB=>R2OH+C6H10O5KPB	1.5E+0008	1.000	25000.0	!	445 KB
DUPLICATE					
R182C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	446 KB
DUPLICATE					
R182C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	447 KB
DUPLICATE					
R182C6H11O6UPB=>R2OH+C6H10O5KPB	4.9E+0007	1.000	17000.0	!	448 KB
DUPLICATE					
R182C6H11O6UPB=>R2OH+C6H10O5KPB	2.5E+0007	1.000	24000.0	!	449 KB
DUPLICATE					
R184C6H11O6UPB=>R2OH+C6H10O5KPB	5.0E+0009	1.000	35500.0	!	450 KB

DUPLICATE					
R184C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	451 KB
DUPLICATE					
R184C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	452 KB
DUPLICATE					
R184C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	453 KB
DUPLICATE					
R185C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	454 KB
DUPLICATE					
R185C6H11O6UPB=>R2OH+C6H10O5KPB	2.9E+0008	1.000	20500.0	!	455 KB
DUPLICATE					
R185C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	456 KB
DUPLICATE					
R185C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0007	1.000	21000.0	!	457 KB
DUPLICATE					
R187C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	458 KB
DUPLICATE					
R187C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	459 KB
DUPLICATE					
R187C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	460 KB
DUPLICATE					
R187C6H11O6UPB=>R2OH+C6H10O5KPB	1.5E+0008	1.000	25000.0	!	461 KB
DUPLICATE					
R188C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	462 KB
DUPLICATE					
R188C6H11O6UPB=>R2OH+C6H10O5KPB	2.9E+0008	1.000	20500.0	!	463 KB
DUPLICATE					
R188C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	464 KB
DUPLICATE					
R188C6H11O6UPB=>R2OH+C6H10O5KPB	2.5E+0007	1.000	24000.0	!	465 KB
DUPLICATE					
R189C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	466 KB
DUPLICATE					
R189C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	467 KB
DUPLICATE					
R189C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	468 KB
DUPLICATE					
R189C6H11O6UPB=>R2OH+C6H10O5KPB	2.5E+0007	1.000	24000.0	!	469 KB
DUPLICATE					
R190C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	470 KB
DUPLICATE					
R190C6H11O6UPB=>R2OH+C6H10O5KPB	8.6E+0008	1.000	28500.0	!	471 KB
DUPLICATE					
R190C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	472 KB
DUPLICATE					
R190C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	473 KB
DUPLICATE					
R191C6H11O6UPB=>R2OH+C6H10O5KPB	5.0E+0009	1.000	35500.0	!	474 KB
DUPLICATE					
R191C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	475 KB
DUPLICATE					
R191C6H11O6UPB=>R2OH+C6H10O5KPB	2.9E+0008	1.000	20500.0	!	476 KB
DUPLICATE					
R191C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	477 KB
DUPLICATE					
R193C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	478 KB
DUPLICATE					
R193C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	479 KB

DUPLICATE						
R193C6H11O6UPB=>R2OH+C6H10O5KPB	4.9E+0007	1.000	17000.0	!	480	KB
DUPLICATE						
R193C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0007	1.000	21000.0	!	481	KB
DUPLICATE						
R195C6H11O6UPB=>R2OH+C6H10O5KPB	1.7E+0009	1.000	27500.0	!	482	KB
DUPLICATE						
R195C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	483	KB
DUPLICATE						
R195C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	484	KB
DUPLICATE						
R195C6H11O6UPB=>R2OH+C6H10O5KPB	1.5E+0008	1.000	25000.0	!	485	KB
DUPLICATE						
R196C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	486	KB
DUPLICATE						
R196C6H11O6UPB=>R2OH+C6H10O5KPB	8.6E+0008	1.000	28500.0	!	487	KB
DUPLICATE						
R196C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	488	KB
DUPLICATE						
R196C6H11O6UPB=>R2OH+C6H10O5KPB	2.9E+0008	1.000	20500.0	!	489	KB
DUPLICATE						
R197C6H11O6UPB=>R2OH+C6H10O5KPB	5.0E+0009	1.000	35500.0	!	490	KB
DUPLICATE						
R197C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	491	KB
DUPLICATE						
R197C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	492	KB
DUPLICATE						
R197C6H11O6UPB=>R2OH+C6H10O5KPB	4.9E+0007	1.000	17000.0	!	493	KB
DUPLICATE						
R199C6H11O6UPB=>R2OH+C6H10O5KPB	3.3E+0009	1.000	32500.0	!	494	KB
DUPLICATE						
R199C6H11O6UPB=>R2OH+C6H10O5KPB	5.7E+0008	1.000	25500.0	!	495	KB
DUPLICATE						
R199C6H11O6UPB=>R2OH+C6H10O5KPB	9.9E+0007	1.000	22000.0	!	496	KB
DUPLICATE						
R199C6H11O6UPB=>R2OH+C6H10O5KPB	8.5E+0006	1.000	16000.0	!	497	KB
DUPLICATE						
R201C3H7O4UP=>R2OH+C3H6O3KP	3.3E+0009	1.000	32500.0	!	498	KB
DUPLICATE						
R201C3H7O4UP=>R2OH+C3H6O3KP	8.6E+0008	1.000	28500.0	!	499	KB
DUPLICATE						
R202C3H7O4UP=>R2OH+C3H6O3KP	1.7E+0009	1.000	27500.0	!	500	KB
DUPLICATE						
R202C3H7O4UP=>R2OH+C3H6O3KP	8.6E+0008	1.000	28500.0	!	501	KB
DUPLICATE						
R204C4H7O5AUP=>R2OH+C4H6O4KAP	3.3E+0009	1.000	30500.0	!	502	KB
DUPLICATE						
R204C4H7O5AUP=>R2OH+C4H6O4KAP	3.3E+0009	1.000	32500.0	!	503	KB
DUPLICATE						
R204C4H7O5AUP=>R2OH+C4H6O4KAP	2.9E+0008	1.000	20500.0	!	504	KB
DUPLICATE						
R205C4H7O5AUP=>R2OH+C4H6O4KAP	1.7E+0009	1.000	27500.0	!	505	KB
DUPLICATE						
R205C4H7O5AUP=>R2OH+C4H6O4KAP	3.3E+0009	1.000	32500.0	!	506	KB
DUPLICATE						
R205C4H7O5AUP=>R2OH+C4H6O4KAP	5.7E+0008	1.000	23500.0	!	507	KB
DUPLICATE						
R206C3H5O5AUP=>R2OH+C3H4O4KAP	1.7E+0009	1.000	27500.0	!	508	KB

DUPLICATE						
R206C3H5O5AUP=>R2OH+C3H4O4KAP	3.3E+0009	1.000	30500.0	!	509	KB
DUPLICATE						
R207C4H7O5AUP=>R2OH+C4H6O4KAP	3.3E+0009	1.000	32500.0	!	510	KB
DUPLICATE						
R207C4H7O5AUP=>R2OH+C4H6O4KAP	5.7E+0008	1.000	25500.0	!	511	KB
DUPLICATE						
R207C4H7O5AUP=>R2OH+C4H6O4KAP	4.9E+0007	1.000	17000.0	!	512	KB
DUPLICATE						
R208C3H5O5AUP=>R2OH+C3H4O4KAP	3.3E+0009	1.000	32500.0	!	513	KB
DUPLICATE						
R208C3H5O5AUP=>R2OH+C3H4O4KAP	2.9E+0008	1.000	20500.0	!	514	KB
DUPLICATE						
R209C4H7O5AUP=>R2OH+C4H6O4KAP	1.7E+0009	1.000	27500.0	!	515	KB
DUPLICATE						
R209C4H7O5AUP=>R2OH+C4H6O4KAP	5.7E+0008	1.000	25500.0	!	516	KB
DUPLICATE						
R209C4H7O5AUP=>R2OH+C4H6O4KAP	4.9E+0007	1.000	17000.0	!	517	KB
DUPLICATE						
R212C5H11O4UP=>R2OH+C5H10O3KP	3.3E+0009	1.000	32500.0	!	518	KB
DUPLICATE						
R212C5H11O4UP=>R2OH+C5H10O3KP	5.7E+0008	1.000	25500.0	!	519	KB
DUPLICATE						
R212C5H11O4UP=>R2OH+C5H10O3KP	9.9E+0007	1.000	22000.0	!	520	KB
DUPLICATE						
R212C5H11O4UP=>R2OH+C5H10O3KP	2.5E+0007	1.000	24000.0	!	521	KB
DUPLICATE						
R213C3H5O5AUP=>R2OH+C3H4O4KAP	1.7E+0009	1.000	27500.0	!	522	KB
DUPLICATE						
R213C3H5O5AUP=>R2OH+C3H4O4KAP	2.9E+0008	1.000	20500.0	!	523	KB
DUPLICATE						
R215C4H7O5AUP=>R2OH+C4H6O4KAP	3.3E+0009	1.000	32500.0	!	524	KB
DUPLICATE						
R215C4H7O5AUP=>R2OH+C4H6O4KAP	2.9E+0008	1.000	20500.0	!	525	KB
DUPLICATE						
R215C4H7O5AUP=>R2OH+C4H6O4KAP	4.9E+0007	1.000	17000.0	!	526	KB
DUPLICATE						
R218C4H7O6UPB=>R2OH+C4H6O5KPB	3.3E+0009	1.000	30500.0	!	527	KB
DUPLICATE						
R218C4H7O6UPB=>R2OH+C4H6O5KPB	3.3E+0009	1.000	32500.0	!	528	KB
DUPLICATE						
R219C4H7O6UPB=>R2OH+C4H6O5KPB	3.3E+0009	1.000	32500.0	!	529	KB
DUPLICATE						
R219C4H7O6UPB=>R2OH+C4H6O5KPB	5.7E+0008	1.000	23500.0	!	530	KB
DUPLICATE						
R220C3H5O6UPB=>R2OH+C3H4O5KPB	3.3E+0009	1.000	30500.0	!	531	KB
R221C4H7O6UPB=>R2OH+C4H6O5KPB	3.3E+0009	1.000	32500.0	!	532	KB
DUPLICATE						
R221C4H7O6UPB=>R2OH+C4H6O5KPB	5.7E+0008	1.000	25500.0	!	533	KB
DUPLICATE						
R222C3H5O6UPB=>R2OH+C3H4O5KPB	3.3E+0009	1.000	32500.0	!	534	KB
R223C4H7O6UPB=>R2OH+C4H6O5KPB	1.7E+0009	1.000	27500.0	!	535	KB
DUPLICATE						
R223C4H7O6UPB=>R2OH+C4H6O5KPB	5.7E+0008	1.000	25500.0	!	536	KB
DUPLICATE						
R225C3H5O6UPB=>R2OH+C3H4O5KPB	1.7E+0009	1.000	27500.0	!	537	KB
R227C4H7O6UPB=>R2OH+C4H6O5KPB	3.3E+0009	1.000	32500.0	!	538	KB
DUPLICATE						

R227C4H7O6UPB=>R2OH+C4H6O5KPB DUPLICATE	2.9E+0008	1.000	20500.0	!	539 KB
R241C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	1.7E+0009	1.000	27500.0	!	540 KB
R241C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	1.7E+0009	1.000	27500.0	!	541 KB
R241C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	8.6E+0008	1.000	28500.0	!	542 KB
R242C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	5.0E+0009	1.000	35500.0	!	543 KB
R242C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	1.7E+0009	1.000	27500.0	!	544 KB
R242C4H7O5AUP=>R2OH+C4H6O4KAP DUPLICATE	2.9E+0008	1.000	20500.0	!	545 KB
R243C4H7O6UPB=>R2OH+C4H6O5KPB DUPLICATE	1.7E+0009	1.000	27500.0	!	546 KB
R243C4H7O6UPB=>R2OH+C4H6O5KPB DUPLICATE	8.6E+0008	1.000	28500.0	!	547 KB
R244C4H7O6UPB=>R2OH+C4H6O5KPB DUPLICATE	5.0E+0009	1.000	35500.0	!	548 KB
R244C4H7O6UPB=>R2OH+C4H6O5KPB DUPLICATE	1.7E+0009	1.000	27500.0	!	549 KB

! beta-scissions :

R19C3H7=>R4CH3+C2H4Z	2.0E+0013	0.000	31000.0	!	DE 550 CN
R20C4H9=>R11C2H5+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 551 CW
R26C5H11=>R4CH3+nC4H8Y	4.0E+0013	0.000	31000.0	!	DE 552 CN
R26C5H11=>R1H+M31C5H10Y	6.0E+0013	0.000	38000.0	!	DE 553 CN
R27C5H11=>R19C3H7+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 554 CW
R27C5H11=>R1H+M32C5H10Z	3.0E+0013	0.000	38000.0	!	DE 555 CN
R28C5H11=>R11C2H5+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 556 CW
R28C5H11=>R1H+M31C5H10Y	3.0E+0013	0.000	38000.0	!	DE 557 CN
R28C5H11=>R1H+M32C5H10Z	3.0E+0013	0.000	39000.0	!	DE 558 CN
R30C6H11OA=>R47C4H7OA+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 559 CW
R30C6H11OA=>R1H+M33C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 560 CN
R31C6H11OA=>R49C3H5OA+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 561 CW
R31C6H11OA=>R1H+M34C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 562 CN
R31C6H11OA=>R1H+M33C6H10OAZ	3.0E+0013	0.000	39000.0	!	DE 563 CN
R32C6H11OA=>R13CH2CHO+nC4H8Y	2.0E+0013	0.000	28700.0	!	DE 564 CW
R32C6H11OA=>R1H+M35C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 565 CN
R32C6H11OA=>R1H+M34C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 566 CN
R32C6H11OA=>R4CH3+C5H8OAZ	2.0E+0013	0.000	31000.0	!	DE 567 CN
R33C6H11OA=>R5CHO+M32C5H10Z	2.0E+0013	0.000	27700.0	!	DE 568
R33C6H11OA=>R1H+M35C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 569 CN
R33C6H11OA=>R1H+M38C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 570 CN
R33C6H11OA=>R11C2H5+C4H6OAZ	2.0E+0013	0.000	28700.0	!	DE 571 CW
R34C6H11OA=>R19C3H7+C2H3CHOZ	2.0E+0013	0.000	28700.0	!	DE 572 CW
R34C6H11OA=>R1H+M38C6H10OAZ	3.0E+0013	0.000	38000.0	!	DE 573 CN
R34C6H11OA=>R1H+M39C6H10OKZ	1.5E+0013	0.000	37500.0	!	DE 574 CN

!Olive

!R35C6H11O2K=>R27C5H11+CO2	9.7E+0015	-1.100	20640.0	!	DE 575
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R35C6H11O2K=>R27C5H11+CO2 5.78E+0014 0.000 16843.5 ! J. Simmie, J. Phys. Chem. A (2012), 116, 4528-4538

!

R36C6H11O2B=>R54C4H7O2B+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 576 CW
R36C6H11O2B=>R1H+M40C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 577 CN
R37C6H11O2B=>R56C3H5O2B+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 578 CW
R37C6H11O2B=>R1H+M41C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 579 CN

R37C6H11O2B=>R1H+M40C6H10O2ZB	3.0E+0013	0.000	39000.0	!	DE 580	CN
R38C6H11O2B=>R23C2H3O2B+nC4H8Y	2.0E+0013	0.000	28700.0	!	DE 581	CW
R38C6H11O2B=>R1H+M42C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 582	CN
R38C6H11O2B=>R1H+M41C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 583	CN
R38C6H11O2B=>R4CH3+C5H8O2ZB	2.0E+0013	0.000	31000.0	!	DE 584	CN
R39C6H11O2B=>R22CO2H+M32C5H10Z	2.1E+0013	0.000	31200.0	!	DE 585	CN
R39C6H11O2B=>R1H+M42C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 586	CN
R39C6H11O2B=>R1H+M45C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 587	CN
R39C6H11O2B=>R11C2H5+C4H6O2ZB	2.0E+0013	0.000	28700.0	!	DE 588	CW
R40C6H11O2B=>R2OH+M39C6H10OKZ	2.1E+0013	0.000	49000.0	!	DE 589	CN
R40C6H11O2B=>R1H+M45C6H10O2ZB	3.0E+0013	0.000	38000.0	!	DE 590	CN
R40C6H11O2B=>R19C3H7+C3H4O2ZB	2.0E+0013	0.000	28700.0	!	DE 591	CW
R47C4H7O2A=>R13CH2CHO+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 592	CW
R49C3H5O2A=>R5CHO+C2H4Z	2.0E+0013	0.000	27700.0	!	DE 593	
R54C4H7O2B=>R23C2H3O2B+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 594	CW
R56C3H5O2B=>R22CO2H+C2H4Z	2.1E+0013	0.000	31200.0	!	DE 595	CN
R60C3H7O2P=>R3OOH+C3H6Y	8.5E+0012	0.000	26000.0	!	DE 596	CR
R62C4H9O2P=>R3OOH+nC4H8Y	8.5E+0012	0.000	26000.0	!	DE 597	CR
R62C4H9O2P=>R4CH3+C3H6O2PZ	2.0E+0013	0.000	31000.0	!	DE 598	CN
R64C4H9O2P=>R16C2H4OOH+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 599	CW
R65C5H11O2P=>R3OOH+M31C5H10Y	8.5E+0012	0.000	26000.0	!	DE 600	CR
R65C5H11O2P=>R11C2H5+C3H6O2PZ	2.0E+0013	0.000	28700.0	!	DE 601	CW
R66C5H11O2P=>R131C3H7O2P+C2H4Z	2.0E+0013	0.000	27700.0	!	DE 602	
R67C5H11O2P=>R3OOH+M32C5H10Z	8.5E+0012	0.000	26000.0	!	DE 603	CR
R67C5H11O2P=>R11C2H5+C3H6O2PZ	2.0E+0013	0.000	28700.0	!	DE 604	CW
R68C5H11O2P=>R4CH3+C4H8O2PZ	2.0E+0013	0.000	31000.0	!	DE 605	CN
R69C5H11O2P=>R16C2H4OOH+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 606	CW
R70C5H11O2P=>R61C3H7O2P+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 607	CW
R71C5H11O2P=>R3OOH+M32C5H10Z	8.5E+0012	0.000	26000.0	!	DE 608	CR
R72C5H11O2P=>R3OOH+M31C5H10Y	8.5E+0012	0.000	26000.0	!	DE 609	CR
R72C5H11O2P=>R4CH3+C4H8O2PZ	2.0E+0013	0.000	31000.0	!	DE 610	CN
DUPLICATE						
R72C5H11O2P=>R4CH3+C4H8O2PZ	2.0E+0013	0.000	31000.0	!	DE 611	CN
DUPLICATE						
R74C5H11O2P=>R140C3H7O2P+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 612	CW
R75C6H11O3AP=>R3OOH+M33C6H10OAZ	8.5E+0012	0.000	26000.0	!	DE 613	CR
R75C6H11O3AP=>R49C3H5OA+C3H6O2PZ	2.0E+0013	0.000	28700.0	!	DE 614	CW
R76C6H11O3AP=>R13CH2CHO+C4H8O2PZ	2.0E+0013	0.000	28700.0	!	DE 615	CW
R77C6H11O3AP=>R16C2H4OOH+C4H6OAZ	2.0E+0013	0.000	28700.0	!	DE 616	CW
R77C6H11O3AP=>R5CHO+C5H10O2PZ	2.0E+0013	0.000	27700.0	!	DE 617	
R78C6H11O3AP=>R61C3H7O2P+C2H3CHOZ	2.0E+0013	0.000	28700.0	!	DE 618	CW
R81C6H11O3AP=>R3OOH+M33C6H10OAZ	8.5E+0012	0.000	26000.0	!	DE 619	CR
R82C6H11O3AP=>R3OOH+M34C6H10OAZ	8.5E+0012	0.000	26000.0	!	DE 620	CR
R82C6H11O3AP=>R13CH2CHO+C4H8O2PZ	2.0E+0013	0.000	28700.0	!	DE 621	CW
R82C6H11O3AP=>R4CH3+C5H8O3APZ	2.0E+0013	0.000	31000.0	!	DE 622	CN
R83C6H11O3AP=>R5CHO+C5H10O2PZ	2.0E+0013	0.000	27700.0	!	DE 623	
R84C6H11O3AP=>R140C3H7O2P+C2H3CHOZ	2.0E+0013	0.000	28700.0	!	DE 624	CW
R87C6H11O3AP=>R3OOH+M34C6H10OAZ	8.5E+0012	0.000	26000.0	!	DE 625	CR
R87C6H11O3AP=>R49C3H5OA+C3H6O2PZ	2.0E+0013	0.000	28700.0	!	DE 626	CW
R88C6H11O3AP=>R157C4H7O3AP+C2H4Z	2.0E+0013	0.000	27700.0	!	DE 627	
R89C6H11O3AP=>R3OOH+M35C6H10OAZ	8.5E+0012	0.000	26000.0	!	DE 628	CR

R89C6H11O3AP=>R5CHO+C5H10O2PZ 2.0E+0013 0.000 27700.0 ! DE 629  
R89C6H11O3AP=>R11C2H5+C4H6O3APZ 2.0E+0013 0.000 28700.0 ! DE 630 CW  
R90C6H11O3AP=>R131C3H7O2P+C2H3CHOZ 2.0E+0013 0.000 27700.0 ! DE 631  
R92C6H11O3AP=>R3OOH+M38C6H10OAZ 8.5E+0012 0.000 26000.0 ! DE 632 CR  
R92C6H11O3AP=>R19C3H7+C3H4O3APZ 2.0E+0013 0.000 28700.0 ! DE 633 CW  
R94C6H11O3AP=>R3OOH+M35C6H10OAZ 8.5E+0012 0.000 26000.0 ! DE 634 CR  
R94C6H11O3AP=>R13CH2CHO+C4H8O2PZ 2.0E+0013 0.000 28700.0 ! DE 635  
CW  
R94C6H11O3AP=>R4CH3+C5H8O3APZ 2.0E+0013 0.000 31000.0 ! DE 636 CN  
R95C6H11O3AP=>R163C3H5O3AP+C3H6Y 2.0E+0013 0.000 27700.0 ! DE 637  
R96C6H11O3AP=>R165C4H7O3AP+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 638  
CW  
R98C6H11O3AP=>R3OOH+M38C6H10OAZ 8.5E+0012 0.000 26000.0 ! DE 639 CR  
R98C6H11O3AP=>R5CHO+C5H10O2PZ 2.0E+0013 0.000 27700.0 ! DE 640  
R98C6H11O3AP=>R11C2H5+C4H6O3APZ 2.0E+0013 0.000 28700.0 ! DE 641 CW  
R99C6H11O3AP=>R4CH3+C5H8O3APZ 2.0E+0013 0.000 31000.0 ! DE 642 CN  
R100C6H11O3AP=>R170C3H5O3AP+C3H6Y 2.0E+0013 0.000 28700.0 ! DE 643  
CW  
R101C6H11O3AP=>R172C4H7O3AP+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 644  
CW  
R102C6H11O4PB=>R3OOH+M40C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 645  
CR  
R102C6H11O4PB=>R56C3H5O2B+C3H6O2PZ 2.0E+0013 0.000 28700.0 ! DE 646  
CW  
R103C6H11O4PB=>R23C2H3O2B+C4H8O2PZ 2.0E+0013 0.000 28700.0 ! DE 647  
CW  
R104C6H11O4PB=>R16C2H4OOH+C4H6O2ZB 2.0E+0013 0.000 28700.0 ! DE 648  
CW  
R104C6H11O4PB=>R22CO2H+C5H10O2PZ 2.1E+0013 0.000 31200.0 ! DE 649  
CN  
R105C6H11O4PB=>R61C3H7O2P+C3H4O2ZB 2.0E+0013 0.000 28700.0 ! DE 650  
CW  
R105C6H11O4PB=>R2OH+C6H10O3KPZ 2.1E+0013 0.000 49000.0 ! DE 651 CN  
R107C6H11O4PB=>R3OOH+M40C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 652  
CR  
R108C6H11O4PB=>R3OOH+M41C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 653  
CR  
R108C6H11O4PB=>R23C2H3O2B+C4H8O2PZ 2.0E+0013 0.000 28700.0 ! DE 654  
CW  
R108C6H11O4PB=>R4CH3+C5H8O4PZB 2.0E+0013 0.000 31000.0 ! DE 655 CN  
R109C6H11O4PB=>R22CO2H+C5H10O2PZ 2.1E+0013 0.000 31200.0 ! DE 656  
CN  
R110C6H11O4PB=>R140C3H7O2P+C3H4O2ZB 2.0E+0013 0.000 28700.0 ! DE  
657 CW  
R110C6H11O4PB=>R2OH+C6H10O3KPZ 2.1E+0013 0.000 49000.0 ! DE 658 CN  
R112C6H11O4PB=>R3OOH+M41C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 659  
CR  
R112C6H11O4PB=>R56C3H5O2B+C3H6O2PZ 2.0E+0013 0.000 28700.0 ! DE 660  
CW  
R113C6H11O4PB=>R186C4H7O4PB+C2H4Z 2.0E+0013 0.000 27700.0 ! DE 661  
R114C6H11O4PB=>R3OOH+M42C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 662  
CR  
R114C6H11O4PB=>R22CO2H+C5H10O2PZ 2.1E+0013 0.000 31200.0 ! DE 663  
CN  
R114C6H11O4PB=>R11C2H5+C4H6O4PZB 2.0E+0013 0.000 28700.0 ! DE 664  
CW  
R115C6H11O4PB=>R131C3H7O2P+C3H4O2ZB 2.0E+0013 0.000 27700.0 ! DE  
665



R115C6H11O4PB=>R2OH+C6H10O3KPZ 2.1E+0013 0.000 49000.0 ! DE 666 CN  
R116C6H11O4PB=>R3OOH+M45C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 667  
CR  
R116C6H11O4PB=>R2OH+C6H10O3KPZ 2.1E+0013 0.000 49000.0 ! DE 668 CN  
R116C6H11O4PB=>R19C3H7+C3H4O4PZB 2.0E+0013 0.000 28700.0 ! DE 669  
CW  
R117C6H11O4PB=>R3OOH+M42C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 670  
CR  
R117C6H11O4PB=>R23C2H3O2B+C4H8O2PZ 2.0E+0013 0.000 28700.0 ! DE 671  
CW  
R117C6H11O4PB=>R4CH3+C5H8O4PZB 2.0E+0013 0.000 31000.0 ! DE 672 CN  
R118C6H11O4PB=>R192C3H5O4PB+C3H6Y 2.0E+0013 0.000 27700.0 ! DE 673  
R119C6H11O4PB=>R194C4H7O4PB+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 674  
CW  
R120C6H11O4PB=>R3OOH+M45C6H10O2ZB 8.5E+0012 0.000 26000.0 ! DE 675  
CR  
R120C6H11O4PB=>R22CO2H+C5H10O2PZ 2.1E+0013 0.000 31200.0 ! DE 676  
CN  
R120C6H11O4PB=>R11C2H5+C4H6O4PZB 2.0E+0013 0.000 28700.0 ! DE 677  
CW  
R121C6H11O4PB=>R4CH3+C5H8O4PZB 2.0E+0013 0.000 31000.0 ! DE 678 CN  
R122C6H11O4PB=>R198C3H5O4PB+C3H6Y 2.0E+0013 0.000 28700.0 ! DE 679  
CW  
R123C6H11O4PB=>R200C4H7O4PB+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 680  
CW  
R131C3H7O2P=>R2OH+C2H5CHO 1.0E+0009 0.000 7500.0 ! DE 681 CW  
R140C3H7O2P=>R3OOH+C3H6Y 8.5E+0012 0.000 26000.0 ! DE 682 CR  
R146C4H7O3AP=>R3OOH+C4H6OAZ 8.5E+0012 0.000 26000.0 ! DE 683 CR  
R146C4H7O3AP=>R5CHO+C3H6O2PZ 2.0E+0013 0.000 27700.0 ! DE 684  
R153C3H5O3AP=>R3OOH+C2H3CHOZ 8.5E+0012 0.000 26000.0 ! DE 685 CR  
R157C4H7O3AP=>R2OH+C4H6O2A2 1.0E+0009 0.000 7500.0 ! DE 686 CW  
R163C3H5O3AP=>R2OH+C3H4O2A2 1.0E+0009 0.000 7500.0 ! DE 687 CW  
R165C4H7O3AP=>R3OOH+C4H6OAZ 8.5E+0012 0.000 26000.0 ! DE 688 CR  
R166C5H11O2P=>R2OH+C5H10OA 1.0E+0009 0.000 7500.0 ! DE 689 CW  
R170C3H5O3AP=>R3OOH+C2H3CHOZ 8.5E+0012 0.000 26000.0 ! DE 690 CR  
R177C4H7O4PB=>R3OOH+C4H6O2ZB 8.5E+0012 0.000 26000.0 ! DE 691 CR  
R177C4H7O4PB=>R22CO2H+C3H6O2PZ 2.1E+0013 0.000 31200.0 ! DE 692 CN  
R178C4H7O4PB=>R2OH+C4H6O3KPZ 2.1E+0013 0.000 49000.0 ! DE 693 CN  
R183C3H5O4PB=>R3OOH+C3H4O2ZB 8.5E+0012 0.000 26000.0 ! DE 694 CR  
R183C3H5O4PB=>R2OH+C3H4O3KPZ 2.1E+0013 0.000 49000.0 ! DE 695 CN  
R186C4H7O4PB=>R2OH+C4H6O3AB 1.0E+0009 0.000 7500.0 ! DE 696 CW  
R192C3H5O4PB=>R2OH+C3H4O3AB 1.0E+0009 0.000 7500.0 ! DE 697 CW  
R194C4H7O4PB=>R3OOH+C4H6O2ZB 8.5E+0012 0.000 26000.0 ! DE 698 CR  
R198C3H5O4PB=>R3OOH+C3H4O2ZB 8.5E+0012 0.000 26000.0 ! DE 699 CR  
R230C4H7O3AP=>R3OOH+C4H6OAZ 8.5E+0012 0.000 26000.0 ! DE 700 CR  
R230C4H7O3AP=>R4CH3+C3H4O3APZ 2.0E+0013 0.000 31000.0 ! DE 701 CN  
R231C4H7O3AP=>R5CHO+C3H6Y 2.0E+0013 0.000 27700.0 ! DE 702  
R234C4H7O3AP=>R3OOH+C4H6OAZ 8.5E+0012 0.000 26000.0 ! DE 703 CR  
R234C4H7O3AP=>R5CHO+C3H6O2PZ 2.0E+0013 0.000 27700.0 ! DE 704  
R235C4H7O3AP=>R4CH3+C2H3CHOZ 2.0E+0013 0.000 31000.0 ! DE 705 CN  
R236C4H7O4PB=>R3OOH+C4H6O2ZB 8.5E+0012 0.000 26000.0 ! DE 706 CR  
R236C4H7O4PB=>R4CH3+C3H4O4PZB 2.0E+0013 0.000 31000.0 ! DE 707 CN  
R236C4H7O4PB=>R2OH+C4H6O3KPZ 2.1E+0013 0.000 49000.0 ! DE 708 CN  
R237C4H7O2B=>R22CO2H+C3H6Y 2.1E+0013 0.000 31200.0 ! DE 709 CN  
R238C3H5O2B=>R2OH+C3H4OKZ 2.1E+0013 0.000 49000.0 ! DE 710 CN  
R239C4H7O4PB=>R3OOH+C4H6O2ZB 8.5E+0012 0.000 26000.0 ! DE 711 CR  
R239C4H7O4PB=>R22CO2H+C3H6O2PZ 2.1E+0013 0.000 31200.0 ! DE 712 CN  
R240C4H7O2B=>R4CH3+C3H4O2ZB 2.0E+0013 0.000 31000.0 ! DE 713 CN

R240C4H7O2B=>R2OH+C4H6OKZ 2.1E+0013 0.000 49000.0 ! DE 714 CN  
R245C5H9O2B=>R49C3H5O2B+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 715 CW  
R246C5H9O2B=>R56C3H5O2B+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 716 CW  
R61C3H7O2P=>R2OH+HCHO+C2H4Z 2.0E+0013 0.000 28700.0 ! DE 717 CW  
R63C4H9O2P=>R2OH+HCHO+C3H6Y 2.0E+0013 0.000 28700.0 ! DE 718 CW  
R68C5H11O2P=>R2OH+HCHO+nC4H8Y 2.0E+0013 0.000 28700.0 ! DE 719 CW  
R73C5H11O2P=>R2OH+CH3CHO+C3H6Y 2.0E+0013 0.000 27700.0 ! DE 720  
R76C6H11O3AP=>R2OH+HCHO+C5H8OAZ 2.0E+0013 0.000 28700.0 ! DE 721 CW  
R83C6H11O3AP=>R2OH+CH3CHO+C4H6OAZ 2.0E+0013 0.000 27700.0 ! DE 722  
R103C6H11O4PB=>R2OH+HCHO+C5H8O2ZB 2.0E+0013 0.000 28700.0 ! DE 723  
CW  
R109C6H11O4PB=>R2OH+CH3CHO+C4H6O2ZB 2.0E+0013 0.000 27700.0 ! DE  
724  
R147C4H7O3AP=>R2OH+HCHO+C2H3CHOZ 2.0E+0013 0.000 28700.0 ! DE 725  
CW  
R178C4H7O4PB=>R2OH+HCHO+C3H4O2ZB 2.0E+0013 0.000 28700.0 ! DE 726  
CW  
R71C5H11O2P=>R2OH+R13CH2CHO+R19C3H7 2.0E+0013 0.000 28700.0 ! DE  
727 CW  
R81C6H11O3AP=>R2OH+R13CH2CHO+R47C4H7OA 2.0E+0013 0.000 28700.0 ! DE  
728 CW  
R107C6H11O4PB=>R2OH+R13CH2CHO+R54C4H7O2B 2.0E+0013 0.000 28700.0 !  
DE 729 CW  
R131C3H7O2P=>R2OH+R13CH2CHO+R4CH3 2.0E+0013 0.000 31000.0 ! DE 730  
CN  
R140C3H7O2P=>R2OH+R13CH2CHO+R4CH3 2.0E+0013 0.000 31000.0 ! DE 731  
CN  
R157C4H7O3AP=>R2OH+R13CH2CHO+R13CH2CHO 2.0E+0013 0.000 28700.0 ! DE  
732 CW  
R163C3H5O3AP=>R2OH+R13CH2CHO+R5CHO 2.0E+0013 0.000 27700.0 ! DE 733  
R165C4H7O3AP=>R2OH+R13CH2CHO+R13CH2CHO 2.0E+0013 0.000 28700.0 ! DE  
734 CW  
R166C5H11O2P=>R2OH+R13CH2CHO+R19C3H7 2.0E+0013 0.000 28700.0 ! DE  
735 CW  
R170C3H5O3AP=>R2OH+R13CH2CHO+R5CHO 2.0E+0013 0.000 27700.0 ! DE 736  
R186C4H7O4PB=>R2OH+R13CH2CHO+R23C2H3O2B 2.0E+0013 0.000 28700.0 !  
DE 737 CW  
R192C3H5O4PB=>R2OH+R13CH2CHO+R22CO2H 2.1E+0013 0.000 31200.0 ! DE  
738 CN  
R194C4H7O4PB=>R2OH+R13CH2CHO+R23C2H3O2B 2.0E+0013 0.000 28700.0 !  
DE 739 CW  
R198C3H5O4PB=>R2OH+R13CH2CHO+R22CO2H 2.1E+0013 0.000 31200.0 ! DE  
740 CN  
! decomposition of R(.)CO free radicals  
!R29C6H11OK=>R27C5H11+B2CO 2.8E+0013 0.000 17150.0 ! DE 741 CN  
R29C6H11OK=>R27C5H11+B2CO 2.8E+0013 0.000 20000.0 !  
!R29C6H11OK=>R27C5H11+B2CO 5.78E+014 0.000 16800.0  
R80C4H7OK=>R19C3H7+B2CO 2.8E+0013 0.000 17150.0 ! DE 742 CN  
R85C6H11O3KP=>R74C5H11O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 743 CN  
R91C6H11O3KP=>R66C5H11O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 744 CN  
R93C6H11O3KP=>R71C5H11O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 745 CN  
R97C6H11O3KP=>R166C5H11O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 746 CN  
R142C6H11O3KP=>R70C5H11O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 747 CN  
R148C4H7O3KP=>R61C3H7O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 748 CN  
R154C3H5O3KP=>R16C2H4OOH+B2CO 2.8E+0013 0.000 17150.0 ! DE 749 CN  
R211C4H7O3KP=>R140C3H7O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 750 CN  
R217C4H7O3KP=>R131C3H7O2P+B2CO 2.8E+0013 0.000 17150.0 ! DE 751 CN  
R232C3H5O3KP=>R2OH+CH3CHO+B2CO 2.8E+0013 0.000 17150.0 ! DE 752 CN

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! decomposition to o-rings :
!Olive
!!R292C6H11O3AP=>gcaprolac+R2OH      3.6E+0009  0.000  7000.0  !
!!R293C6H11O3AP=>dcaprolac+R2OH      1.7E+0008  0.000  1950.0  !
R292C6H11O3AP=>gcaprolac+R2OH      1.57E+0008  0.270  7800.0  !Cord Ea was
7800 A/10
R292C6H11O3AP=>nC4H8Y+R2OH+HCHO+B2CO  3.3E+013  0.000  22500.0  !Exgas
allylique
R293C6H11O3AP=>dcaprolac+R2OH      2.2E+0008  0.110  10400.0  !Cord
!R292C6H11O3AP=>gcaprolac+R2OH      4.82E+0007  0.94  9000.0  !Villano
!R293C6H11O3AP=>dcaprolac+R2OH      3.05E+0007  0.83  8800.0  !Villano
!R292C6H11O3AP=>gcaprolac+R2OH      4.160E+10  0.0000  11501.0
!Galway
!R293C6H11O3AP=>dcaprolac+R2OH      7.800E+09  0.0000  11137.0
!Galway
!gcaprolac+R2OH=>H2O+2B2CO+C2H4Z+R11C2H5  9.1E+0006  2.000  -765.0
!as M10
!dcaprolac+R2OH=>H2O+2B2CO+C2H4Z+R11C2H5  9.1E+0006  2.000  -765.0
!as M10
!
R60C3H7O2P=>R2OH+C3H6OE#3      6.1E+0011  0.000  17950.0  ! OR 753 CR
R61C3H7O2P=>R2OH+C3H6OE#4      9.2E+0010  0.000  16600.0  ! OR 754 CR
R62C4H9O2P=>R2OH+C4H8OE#3      6.1E+0011  0.000  17950.0  ! OR 755 CR
R63C4H9O2P=>R2OH+C4H8OE#4      9.2E+0010  0.000  16600.0  ! OR 756 CR
R64C4H9O2P=>R2OH+C4H8OE#5      3.6E+0009  0.000  7000.0  ! OR 757 CR
R65C5H11O2P=>R2OH+M7C5H10OE#3  6.1E+0011  0.000  17950.0  ! OR 758 CR
R66C5H11O2P=>R2OH+M8C5H10OE#4  9.2E+0010  0.000  16600.0  ! OR 759 CR
R67C5H11O2P=>R2OH+M9C5H10OE#3  6.1E+0011  0.000  17950.0  ! OR 760 CR
R68C5H11O2P=>R2OH+M8C5H10OE#4  9.2E+0010  0.000  16600.0  ! OR 761 CR
R69C5H11O2P=>R2OH+M10C5H10OE#5  3.6E+0009  0.000  7000.0  ! OR 762 CR
R70C5H11O2P=>R2OH+M11C5H10OE#6  1.7E+0008  0.000  1950.0  ! OR 763 CR
R71C5H11O2P=>R2OH+M9C5H10OE#3  6.1E+0011  0.000  17950.0  ! OR 764 CR
R72C5H11O2P=>R2OH+M7C5H10OE#3  6.1E+0011  0.000  17950.0  ! OR 765 CR
R73C5H11O2P=>R2OH+M12C5H10OE#4  9.2E+0010  0.000  16600.0  ! OR 766 CR
R74C5H11O2P=>R2OH+M10C5H10OE#5  3.6E+0009  0.000  7000.0  ! OR 767 CR
R75C6H11O3AP=>R2OH+M13C6H10O2E#3A  6.1E+0011  0.000  17950.0  ! OR 768
CR
R76C6H11O3AP=>R2OH+M14C6H10O2E#4A  9.2E+0010  0.000  16600.0  ! OR 769
CR
R77C6H11O3AP=>R2OH+M15C6H10O2E#5A  3.6E+0009  0.000  7000.0  ! OR 770
CR
R78C6H11O3AP=>R2OH+M16C6H10O2E#6A  1.7E+0008  0.000  1950.0  ! OR 771
CR
R81C6H11O3AP=>R2OH+M13C6H10O2E#3A  6.1E+0011  0.000  17950.0  ! OR 772
CR
R82C6H11O3AP=>R2OH+M17C6H10O2E#3A  6.1E+0011  0.000  17950.0  ! OR 773
CR
R83C6H11O3AP=>R2OH+M18C6H10O2E#4A  9.2E+0010  0.000  16600.0  ! OR 774
CR
R84C6H11O3AP=>R2OH+M19C6H10O2E#5A  3.6E+0009  0.000  7000.0  ! OR 775
CR
R87C6H11O3AP=>R2OH+M17C6H10O2E#3A  6.1E+0011  0.000  17950.0  ! OR 776
CR
R88C6H11O3AP=>R2OH+M14C6H10O2E#4A  9.2E+0010  0.000  16600.0  ! OR 777
CR
R89C6H11O3AP=>R2OH+M20C6H10O2E#3A  6.1E+0011  0.000  17950.0  ! OR 778
CR

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R90C6H11O3AP=>R2OH+M21C6H10O2E#4A CR	9.2E+0010	0.000	16600.0	! OR 779
R92C6H11O3AP=>R2OH+M22C6H10O2E#3A CR	6.1E+0011	0.000	17950.0	! OR 780
R94C6H11O3AP=>R2OH+M20C6H10O2E#3A CR	6.1E+0011	0.000	17950.0	! OR 781
R95C6H11O3AP=>R2OH+M18C6H10O2E#4A CR	9.2E+0010	0.000	16600.0	! OR 782
R96C6H11O3AP=>R2OH+M15C6H10O2E#5A CR	3.6E+0009	0.000	7000.0	! OR 783
R98C6H11O3AP=>R2OH+M22C6H10O2E#3A CR	6.1E+0011	0.000	17950.0	! OR 784
R99C6H11O3AP=>R2OH+M21C6H10O2E#4A CR	9.2E+0010	0.000	16600.0	! OR 785
R100C6H11O3AP=>R2OH+M19C6H10O2E#5A CR	3.6E+0009	0.000	7000.0	! OR 786
R101C6H11O3AP=>R2OH+M16C6H10O2E#6A CR	1.7E+0008	0.000	1950.0	! OR 787
R102C6H11O4PB=>R2OH+M23C6H10O3E#3LK 788 CR	6.1E+0011	0.000	17950.0	! OR
R103C6H11O4PB=>R2OH+M24C6H10O3E#4LK 789 CR	9.2E+0010	0.000	16600.0	! OR
R104C6H11O4PB=>R2OH+M25C6H10O3E#5LK CR	3.6E+0009	0.000	7000.0	! OR 790
R105C6H11O4PB=>R2OH+M26C6H10O3E#6LK CR	1.7E+0008	0.000	1950.0	! OR 791
R107C6H11O4PB=>R2OH+M23C6H10O3E#3LK 792 CR	6.1E+0011	0.000	17950.0	! OR
R108C6H11O4PB=>R2OH+M27C6H10O3E#3LK 793 CR	6.1E+0011	0.000	17950.0	! OR
R109C6H11O4PB=>R2OH+M28C6H10O3E#4LK 794 CR	9.2E+0010	0.000	16600.0	! OR
R110C6H11O4PB=>R2OH+M29C6H10O3E#5LK CR	3.6E+0009	0.000	7000.0	! OR 795
R112C6H11O4PB=>R2OH+M27C6H10O3E#3LK 796 CR	6.1E+0011	0.000	17950.0	! OR
R113C6H11O4PB=>R2OH+M24C6H10O3E#4LK 797 CR	9.2E+0010	0.000	16600.0	! OR
R114C6H11O4PB=>R2OH+M30C6H10O3E#3LK 798 CR	6.1E+0011	0.000	17950.0	! OR
R115C6H11O4PB=>R2OH+M31C6H10O3E#4LK 799 CR	9.2E+0010	0.000	16600.0	! OR
R116C6H11O4PB=>R2OH+M32C6H10O3E#3LK 800 CR	6.1E+0011	0.000	17950.0	! OR
R117C6H11O4PB=>R2OH+M30C6H10O3E#3LK 801 CR	6.1E+0011	0.000	17950.0	! OR
R118C6H11O4PB=>R2OH+M28C6H10O3E#4LK 802 CR	9.2E+0010	0.000	16600.0	! OR
R119C6H11O4PB=>R2OH+M25C6H10O3E#5LK CR	3.6E+0009	0.000	7000.0	! OR 803
R120C6H11O4PB=>R2OH+M32C6H10O3E#3LK 804 CR	6.1E+0011	0.000	17950.0	! OR
R121C6H11O4PB=>R2OH+M31C6H10O3E#4LK 805 CR	9.2E+0010	0.000	16600.0	! OR
R122C6H11O4PB=>R2OH+M29C6H10O3E#5LK CR	3.6E+0009	0.000	7000.0	! OR 806
R123C6H11O4PB=>R2OH+M26C6H10O3E#6LK CR	1.7E+0008	0.000	1950.0	! OR 807

R140C3H7O2P=>R2OH+C3H6OE#3 6.1E+0011 0.000 17950.0 ! OR 808 CR  
R146C4H7O3AP=>R2OH+C4H6O2E#3A 6.1E+0011 0.000 17950.0 ! OR 809 CR  
R147C4H7O3AP=>R2OH+C4H6O2E#4A 9.2E+0010 0.000 16600.0 ! OR 810 CR  
R153C3H5O3AP=>R2OH+C3H4O2E#3A 6.1E+0011 0.000 17950.0 ! OR 811 CR  
R165C4H7O3AP=>R2OH+C4H6O2E#3A 6.1E+0011 0.000 17950.0 ! OR 812 CR  
R170C3H5O3AP=>R2OH+C3H4O2E#3A 6.1E+0011 0.000 17950.0 ! OR 813 CR  
R172C4H7O3AP=>R2OH+C4H6O2E#4A 9.2E+0010 0.000 16600.0 ! OR 814 CR  
R177C4H7O4PB=>R2OH+C4H6O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 815 CR  
R178C4H7O4PB=>R2OH+C4H6O3E#4LK 9.2E+0010 0.000 16600.0 ! OR 816 CR  
R183C3H5O4PB=>R2OH+C3H4O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 817 CR  
R194C4H7O4PB=>R2OH+C4H6O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 818 CR  
R198C3H5O4PB=>R2OH+C3H4O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 819 CR  
R200C4H7O4PB=>R2OH+C4H6O3E#4LK 9.2E+0010 0.000 16600.0 ! OR 820 CR  
R230C4H7O3AP=>R2OH+C4H6O2E#3A 6.1E+0011 0.000 17950.0 ! OR 821 CR  
R234C4H7O3AP=>R2OH+C4H6O2E#3A 6.1E+0011 0.000 17950.0 ! OR 822 CR  
R236C4H7O4PB=>R2OH+C4H6O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 823 CR  
R239C4H7O4PB=>R2OH+C4H6O3E#3LK 6.1E+0011 0.000 17950.0 ! OR 824 CR

! oxidations :

R19C3H7+O2=>C3H6Y+R3OOH 2.8E+0012 0.000 5000.0 ! OX 825 CW  
R20C4H9+O2=>nC4H8Y+R3OOH 2.8E+0012 0.000 5000.0 ! OX 826 CW  
R26C5H11+O2=>M31C5H10Y+R3OOH 3.9E+0012 0.000 5000.0 ! OX 827 CN  
R27C5H11+O2=>M32C5H10Z+R3OOH 1.9E+0012 0.000 5000.0 ! OX 828 CN  
R28C5H11+O2=>M31C5H10Y+R3OOH 1.9E+0012 0.000 5000.0 ! OX 829 CN  
R28C5H11+O2=>M32C5H10Z+R3OOH 8.1E+0011 0.000 5000.0 ! OX 830 CN  
R229C3H7+O2=>C3H6Y+R3OOH 2.3E+0012 0.000 5000.0 ! OX 831 CW

!1-hexanol (added by Olivier because missing in the generation)

!R33C6H13O+O2=C6H12OA-1+R3OOH 1.9E+0012 0.000 5000.0  
!R32C6H13OL+O2=C6H12OA-1+R3OOH 1.9E+0012 0.000 5000.0  
!R32C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 694 CN  
!R34C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 696 CN  
!R35C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 697 CN  
! DUPLICATE  
!R35C6H13OL+O2=C6H12OLZ+R3OOH 8.1E+0011 0.000 5000.0 ! OX 698 CN  
! DUPLICATE  
!R36C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 699 CN  
! DUPLICATE  
!R36C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 700 CN  
! DUPLICATE  
!R37C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 701 CN  
! DUPLICATE  
!R37C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 702 CN  
! DUPLICATE  
!R38C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 703 CN  
! DUPLICATE  
!R38C6H13OL+O2=C6H12OLZ+R3OOH 1.9E+0012 0.000 5000.0 ! OX 704 CN  
! DUPLICATE

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

! metathesis :

!Olive

C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R29C6H11OK 0.75E+0011 0.000 2900.0  
!  
C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R30C6H11OA 1.6E+0012 0.000 7300.0  
!

C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R31C6H11OA	1.5E+0012	0.000	4500.0	
!				
C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R32C6H11OA	1.5E+0012	0.000	4500.0	
!				
C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R33C6H11OA	1.5E+0012	0.000	4500.0	
!				
C6H12OA-1+R35C6H11O2K=C6H12O2B-1+R34C6H11OA	1.5E+0012	0.000	4500.0	
!				
!				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R29C6H11OK	1.5E+0011	0.000		
15000.0 !				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R30C6H11OA	6.0E+0011	0.000		
20000.0 !				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R31C6H11OA	3.0E+0011	0.000		
17500.0 !				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R32C6H11OA	3.0E+0011	0.000		
17500.0 !				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R33C6H11OA	3.0E+0011	0.000		
17500.0 !				
C6H12OA-1+R290C6H11O3AU=>C6H11OKOOH+R34C6H11OA	3.0E+0011	0.000		
17500.0 !				
!				

!H-atom abstractions by O

B1O+C5H12-1=>R2OH+R26C5H11	2.6E+0013	0.000	5200.0	! ME 832 CW
B1O+C5H12-1=>R2OH+R27C5H11	1.0E+0014	0.000	7850.0	! ME 833 CW
B1O+C5H12-1=>R2OH+R28C5H11	5.2E+0013	0.000	5200.0	! ME 834 CW
B1O+C6H12OA-1=>R2OH+R29C6H11OK	1.0E+0013	0.000	3280.0	! ME 835 CW
B1O+C6H12OA-1=>R2OH+R30C6H11OA	5.1E+0013	0.000	7850.0	! ME 836 CW
B1O+C6H12OA-1=>R2OH+R31C6H11OA	2.6E+0013	0.000	5200.0	! ME 837 CW
B1O+C6H12OA-1=>R2OH+R32C6H11OA	2.6E+0013	0.000	5200.0	! ME 838 CW
B1O+C6H12OA-1=>R2OH+R33C6H11OA	2.6E+0013	0.000	5200.0	! ME 839 CW
B1O+C6H12OA-1=>R2OH+R34C6H11OA	2.6E+0013	0.000	5200.0	! ME 840 CW
B1O+C6H12O2B-1=>R2OH+R35C6H11O2K	1.3E+0006	2.000	5025.0	! ME 841 CW
B1O+C6H12O2B-1=>R2OH+R36C6H11O2B	5.1E+0013	0.000	7850.0	! ME 842 CW
B1O+C6H12O2B-1=>R2OH+R37C6H11O2B	2.6E+0013	0.000	5200.0	! ME 843 CW
B1O+C6H12O2B-1=>R2OH+R38C6H11O2B	2.6E+0013	0.000	5200.0	! ME 844 CW
B1O+C6H12O2B-1=>R2OH+R39C6H11O2B	2.6E+0013	0.000	5200.0	! ME 845 CW
B1O+C6H12O2B-1=>R2OH+R40C6H11O2B	3.4E+0008	1.500	620.0	! ME 846 CW
!B1O+C6H14OL-1=>R2OH+R32C6H13OL	3.9E+0013	0.000	5200.0	! ME 1112 CW
B1O+C6H14OL-1=>R2OH+R32C6H13OL	1.45e05	2.500	876.0	!TogbÃ© 2010
B1O+C6H14OL-1=>R2OH+R33C6H13O	1.3E+0006	2.000	5025.0	! ME 1113 CW
B1O+C6H14OL-1=>R2OH+R34C6H13OL	5.1E+0013	0.000	7850.0	! ME 1114 CW
B1O+C6H14OL-1=>R2OH+R35C6H13OL	2.6E+0013	0.000	5200.0	! ME 1115 CW
B1O+C6H14OL-1=>R2OH+R36C6H13OL	2.6E+0013	0.000	5200.0	! ME 1116 CW
B1O+C6H14OL-1=>R2OH+R37C6H13OL	2.6E+0013	0.000	5200.0	! ME 1117 CW
B1O+C6H14OL-1=>R2OH+R38C6H13OL	2.6E+0013	0.000	5200.0	! ME 1118 CW

!H-atom abstractions by H

C5H12-1+R1H=>H2+R26C5H11	9.0E+0006	2.000	5000.0	! ME 847 CW
C5H12-1+R1H=>H2+R27C5H11	5.7E+0007	2.000	7700.0	! ME 848 CW
C5H12-1+R1H=>H2+R28C5H11	1.8E+0007	2.000	5000.0	! ME 849 CW
C6H12OA-1+R1H=>H2+R29C6H11OK	4.2E+0006	2.000	2400.0	! ME 850 CN
C6H12OA-1+R1H=>H2+R30C6H11OA	2.9E+0007	2.000	7700.0	! ME 851 CW
C6H12OA-1+R1H=>H2+R31C6H11OA	9.0E+0006	2.000	5000.0	! ME 852 CW
C6H12OA-1+R1H=>H2+R32C6H11OA	9.0E+0006	2.000	5000.0	! ME 853 CW
C6H12OA-1+R1H=>H2+R33C6H11OA	9.0E+0006	2.000	5000.0	! ME 854 CW

C6H12OA-1+R1H=>H2+R34C6H11OA	9.0E+0006	2.000	5000.0	! ME 855 CW
C6H12O2B-1+R1H=>H2+R35C6H11O2K	2.4E+0006	2.000	6525.0	! ME 856 CN
C6H12O2B-1+R1H=>H2+R36C6H11O2B	2.9E+0007	2.000	7700.0	! ME 857 CW
C6H12O2B-1+R1H=>H2+R37C6H11O2B	9.0E+0006	2.000	5000.0	! ME 858 CW
C6H12O2B-1+R1H=>H2+R38C6H11O2B	9.0E+0006	2.000	5000.0	! ME 859 CW
C6H12O2B-1+R1H=>H2+R39C6H11O2B	9.0E+0006	2.000	5000.0	! ME 860 CW
C6H12O2B-1+R1H=>H2+R40C6H11O2B	4.8E+0008	1.500	2980.0	! ME 861 CN
!C6H14OL-1+R1H=>H2+R32C6H13OL	1.3E+0007	2.000	5000.0	! ME 1128 CN
C6H14OL-1+R1H=>H2+R32C6H13OL	1.79e5	2.5	3420.0	!TogbÄ© 2010
C6H14OL-1+R1H=>H2+R33C6H13O	2.4E+0006	2.000	6525.0	! ME 1129 CN
C6H14OL-1+R1H=>H2+R34C6H13OL	2.9E+0007	2.000	7700.0	! ME 1130 CW
C6H14OL-1+R1H=>H2+R35C6H13OL	9.0E+0006	2.000	5000.0	! ME 1131 CW
C6H14OL-1+R1H=>H2+R36C6H13OL	9.0E+0006	2.000	5000.0	! ME 1132 CW
C6H14OL-1+R1H=>H2+R37C6H13OL	9.0E+0006	2.000	5000.0	! ME 1133 CW
C6H14OL-1+R1H=>H2+R38C6H13OL	9.0E+0006	2.000	5000.0	! ME 1134 CW

!H-atom abstractions by OH

C5H12-1+R2OH=>H2O+R26C5H11	2.6E+0006	2.000	-765.0	! ME 862 CW
C5H12-1+R2OH=>H2O+R27C5H11	5.4E+0006	2.000	450.0	! ME 863 CW
C5H12-1+R2OH=>H2O+R28C5H11	5.2E+0006	2.000	-765.0	! ME 864 CW
!C6H12OA-1+R2OH=>H2O+R29C6H11OK	1.1E+0006	2.000	-1865.0	! ME 865 CW
C6H12OA-1+R2OH=>H2O+R30C6H11OA	2.7E+0006	2.000	450.0	! ME 866 CW
C6H12OA-1+R2OH=>H2O+R31C6H11OA	2.6E+0006	2.000	-765.0	! ME 867 CW
C6H12OA-1+R2OH=>H2O+R32C6H11OA	2.6E+0006	2.000	-765.0	! ME 868 CW
C6H12OA-1+R2OH=>H2O+R33C6H11OA	2.6E+0006	2.000	-765.0	! ME 869 CW
!C6H12OA-1+R2OH=>H2O+R34C6H11OA	2.6E+0006	2.000	-765.0	! ME 870 CW
C6H12OA-1+R2OH=>H2O+R34C6H11OA	2.2E+0006	2.000	-1865.0	!like

tertiary

!

C6H12OA-1+R2OH=>H2O+R29C6H11OK	+3.3700000E+012	+0.0000000E+000	-	
6.1900000E+002	!			
!C6H12OA-1+R2OH=>H2O+R30C6H11OA	+2.7320000E+007	+1.8130000E+000		
+8.6840000E+002	!			
!C6H12OA-1+R2OH=>H2O+R31C6H11OA	+1.4110000E+010	+9.3500000E-001		
+5.0470000E+002	!			
!C6H12OA-1+R2OH=>H2O+R32C6H11OA	+1.4110000E+010	+9.3500000E-001		
+5.0470000E+002	!			
!C6H12OA-1+R2OH=>H2O+R33C6H11OA	+1.4110000E+010	+9.3500000E-001		
+5.0470000E+002	!			
!C6H12OA-1+R2OH=>H2O+R34C6H11OA	+1.4110000E+010	+9.3500000E-001		
+5.0470000E+002	!			

!

C6H12O2B-1+R2OH=>H2O+R35C6H11O2K	4.0E+0005	2.000	-475.0	! ME 871 CN
C6H12O2B-1+R2OH=>H2O+R36C6H11O2B	2.7E+0006	2.000	450.0	! ME 872 CW
C6H12O2B-1+R2OH=>H2O+R37C6H11O2B	2.6E+0006	2.000	-765.0	! ME 873 CW
C6H12O2B-1+R2OH=>H2O+R38C6H11O2B	2.6E+0006	2.000	-765.0	! ME 874 CW
C6H12O2B-1+R2OH=>H2O+R39C6H11O2B	2.6E+0006	2.000	-765.0	! ME 875 CW
C6H12O2B-1+R2OH=>H2O+R40C6H11O2B	2.4E+0006	2.000	-2450.0	! ME 876

CN

!C6H14OL-1+R2OH=>H2O+R32C6H13OL	3.9E+0006	2.000	-765.0	! ME 1144 CN
C6H14OL-1+R2OH=>H2O+R32C6H13OL	1.31e5	2.4	-1456.0	!TogbÄ© 2010
C6H14OL-1+R2OH=>H2O+R33C6H13O	4.0E+0005	2.000	-475.0	! ME 1145 CN
C6H14OL-1+R2OH=>H2O+R34C6H13OL	2.7E+0006	2.000	450.0	! ME 1146 CW
C6H14OL-1+R2OH=>H2O+R35C6H13OL	2.6E+0006	2.000	-765.0	! ME 1147 CW
C6H14OL-1+R2OH=>H2O+R36C6H13OL	2.6E+0006	2.000	-765.0	! ME 1148 CW
C6H14OL-1+R2OH=>H2O+R37C6H13OL	2.6E+0006	2.000	-765.0	! ME 1149 CW
C6H14OL-1+R2OH=>H2O+R38C6H13OL	2.6E+0006	2.000	-765.0	! ME 1150 CW

!H-atom abstractions by HO2

C5H12-1+R3OOH=>H2O2+R26C5H11	4.0E+0011	0.000	15500.0	! ME 877	CN
C5H12-1+R3OOH=>H2O2+R27C5H11	1.2E+0012	0.000	17000.0	! ME 878	CN
C5H12-1+R3OOH=>H2O2+R28C5H11	8.0E+0011	0.000	15500.0	! ME 879	CN
C6H12OA-1+R3OOH=>H2O2+R29C6H11OK	0.950E+004		2.70	11520.0	
C6H12OA-1+R3OOH=>H2O2+R30C6H11OA	6.0E+0011	0.000	17000.0	! ME 880	CN
C6H12OA-1+R3OOH=>H2O2+R31C6H11OA	4.0E+0011	0.000	15500.0	! ME 881	CN
C6H12OA-1+R3OOH=>H2O2+R32C6H11OA	4.0E+0011	0.000	15500.0	! ME 882	CN
C6H12OA-1+R3OOH=>H2O2+R33C6H11OA	4.0E+0011	0.000	15500.0	! ME 883	CN
C6H12OA-1+R3OOH=>H2O2+R34C6H11OA	4.0E+0011	0.000	15500.0	! ME 884	CN
C6H12O2B-1+R3OOH=>H2O2+R35C6H11O2K	5.4E+0004	2.000	15025.0	! ME 885	CN
C6H12O2B-1+R3OOH=>H2O2+R36C6H11O2B	6.0E+0011	0.000	17000.0	! ME 886	CN
C6H12O2B-1+R3OOH=>H2O2+R37C6H11O2B	4.0E+0011	0.000	15500.0	! ME 887	CN
C6H12O2B-1+R3OOH=>H2O2+R38C6H11O2B	4.0E+0011	0.000	15500.0	! ME 888	CN
C6H12O2B-1+R3OOH=>H2O2+R39C6H11O2B	4.0E+0011	0.000	15500.0	! ME 889	CN
C6H12O2B-1+R3OOH=>H2O2+R40C6H11O2B	2.8E+0004	2.690	15000.0	! ME 890	CR
C5H12-1+R4CH3=>CH4+R26C5H11	2.0E+0011	0.000	9600.0	! ME 891	CN
C5H12-1+R4CH3=>CH4+R27C5H11	6.0E-0001	4.000	8200.0	! ME 892	CN
C5H12-1+R4CH3=>CH4+R28C5H11	4.0E+0011	0.000	9600.0	! ME 893	CN
C6H12OA-1+R4CH3=>CH4+R29C6H11OK	1.0E+0011	0.000	7900.0	! ME 894	CW
C6H12OA-1+R4CH3=>CH4+R30C6H11OA	3.0E-0001	4.000	8200.0	! ME 895	CN
C6H12OA-1+R4CH3=>CH4+R31C6H11OA	2.0E+0011	0.000	9600.0	! ME 896	CN
C6H12OA-1+R4CH3=>CH4+R32C6H11OA	2.0E+0011	0.000	9600.0	! ME 897	CN
C6H12OA-1+R4CH3=>CH4+R33C6H11OA	2.0E+0011	0.000	9600.0	! ME 898	CN
C6H12OA-1+R4CH3=>CH4+R34C6H11OA	2.0E+0011	0.000	9600.0	! ME 899	CN
C6H12O2B-1+R4CH3=>CH4+R35C6H11O2K	4.2E+0004	2.000	3925.0	! ME 900	
C6H12O2B-1+R4CH3=>CH4+R36C6H11O2B	3.0E-0001	4.000	8200.0	! ME 901	CN
C6H12O2B-1+R4CH3=>CH4+R37C6H11O2B	2.0E+0011	0.000	9600.0	! ME 902	CN
C6H12O2B-1+R4CH3=>CH4+R38C6H11O2B	2.0E+0011	0.000	9600.0	! ME 903	CN
C6H12O2B-1+R4CH3=>CH4+R39C6H11O2B	2.0E+0011	0.000	9600.0	! ME 904	CN
C6H12O2B-1+R4CH3=>CH4+R40C6H11O2B	1.6E+0006	1.870	6510.0	! ME 905	CR
C5H12-1+R5CHO=>HCHO+R26C5H11	1.0E+0007	1.900	17000.0	! ME 906	CN
C5H12-1+R5CHO=>HCHO+R27C5H11	2.0E+0005	2.500	18500.0	! ME 907	CN
C5H12-1+R5CHO=>HCHO+R28C5H11	2.2E+0007	1.900	17000.0	! ME 908	CN
C6H12OA-1+R5CHO=>HCHO+R30C6H11OA	1.0E+0005	2.500	18500.0	! ME 909	CN
C6H12OA-1+R5CHO=>HCHO+R31C6H11OA	1.0E+0007	1.900	17000.0	! ME 910	CN
C6H12OA-1+R5CHO=>HCHO+R32C6H11OA	1.0E+0007	1.900	17000.0	! ME 911	CN



C6H12OA-1+R5CHO=>HCHO+R33C6H11OA CN	1.0E+0007	1.900	17000.0	! ME 912
C6H12OA-1+R5CHO=>HCHO+R34C6H11OA CN	1.0E+0007	1.900	17000.0	! ME 913
C6H12O2B-1+R5CHO=>HCHO+R35C6H11O2K	1.2E+0005	2.000	15525.0	! ME 914
C6H12O2B-1+R5CHO=>HCHO+R36C6H11O2B CN	1.0E+0005	2.500	18500.0	! ME 915
C6H12O2B-1+R5CHO=>HCHO+R37C6H11O2B CN	1.0E+0007	1.900	17000.0	! ME 916
C6H12O2B-1+R5CHO=>HCHO+R38C6H11O2B CN	1.0E+0007	1.900	17000.0	! ME 917
C6H12O2B-1+R5CHO=>HCHO+R39C6H11O2B CN	1.0E+0007	1.900	17000.0	! ME 918
C6H12O2B-1+R5CHO=>HCHO+R40C6H11O2B CR	6.8E+0004	2.500	13500.0	! ME 919
C5H12-1+R6CH2OH=>CH3OH+R26C5H11	6.0E+0001	2.950	12000.0	! ME 920 CN
C5H12-1+R6CH2OH=>CH3OH+R27C5H11	2.0E+0002	2.950	14000.0	! ME 921 CN
C5H12-1+R6CH2OH=>CH3OH+R28C5H11	1.2E+0002	2.950	12000.0	! ME 922 CN
C6H12OA-1+R6CH2OH=>CH3OH+R30C6H11OA 923 CN	9.9E+0001	2.950	14000.0	! ME
C6H12OA-1+R6CH2OH=>CH3OH+R31C6H11OA 924 CN	6.0E+0001	2.950	12000.0	! ME
C6H12OA-1+R6CH2OH=>CH3OH+R32C6H11OA 925 CN	6.0E+0001	2.950	12000.0	! ME
C6H12OA-1+R6CH2OH=>CH3OH+R33C6H11OA 926 CN	6.0E+0001	2.950	12000.0	! ME
C6H12OA-1+R6CH2OH=>CH3OH+R34C6H11OA 927 CN	6.0E+0001	2.950	12000.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R35C6H11O2K 928	2.8E+0004	2.000	14025.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R36C6H11O2B 929 CN	9.9E+0001	2.950	14000.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R37C6H11O2B 930 CN	6.0E+0001	2.950	12000.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R38C6H11O2B 931 CN	6.0E+0001	2.950	12000.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R39C6H11O2B 932 CN	6.0E+0001	2.950	12000.0	! ME
C6H12O2B-1+R6CH2OH=>CH3OH+R40C6H11O2B 933 CR	2.4E+0002	2.760	10800.0	! ME
C5H12-1+R7CH3O=>CH3OH+R26C5H11	1.5E+0011	0.000	4500.0	! ME 934 CN
C5H12-1+R7CH3O=>CH3OH+R27C5H11	3.2E+0011	0.000	7300.0	! ME 935 CN
C5H12-1+R7CH3O=>CH3OH+R28C5H11	2.9E+0011	0.000	4500.0	! ME 936 CN
C6H12OA-1+R7CH3O=>CH3OH+R30C6H11OA CN	1.6E+0011	0.000	7300.0	! ME 937
C6H12OA-1+R7CH3O=>CH3OH+R31C6H11OA CN	1.5E+0011	0.000	4500.0	! ME 938
C6H12OA-1+R7CH3O=>CH3OH+R32C6H11OA CN	1.5E+0011	0.000	4500.0	! ME 939
C6H12OA-1+R7CH3O=>CH3OH+R33C6H11OA CN	1.5E+0011	0.000	4500.0	! ME 940
C6H12OA-1+R7CH3O=>CH3OH+R34C6H11OA CN	1.5E+0011	0.000	4500.0	! ME 941
C6H12O2B-1+R7CH3O=>CH3OH+R35C6H11O2K 942	4.2E+0004	2.000	3925.0	! ME
C6H12O2B-1+R7CH3O=>CH3OH+R36C6H11O2B 943 CN	1.6E+0011	0.000	7300.0	! ME

C6H12O2B-1+R7CH3O=>CH3OH+R37C6H11O2B 944 CN	1.5E+0011	0.000	4500.0	! ME
C6H12O2B-1+R7CH3O=>CH3OH+R38C6H11O2B 945 CN	1.5E+0011	0.000	4500.0	! ME
C6H12O2B-1+R7CH3O=>CH3OH+R39C6H11O2B 946 CN	1.5E+0011	0.000	4500.0	! ME
C6H12O2B-1+R7CH3O=>CH3OH+R40C6H11O2B 947 CR	4.6E+0010	0.000	2900.0	! ME
C5H12-1+R8CH3OO=>CH3OOH+R26C5H11 CN	3.0E+0012	0.000	17500.0	! ME 948
C5H12-1+R8CH3OO=>CH3OOH+R27C5H11 CN	1.2E+0013	0.000	20000.0	! ME 949
C5H12-1+R8CH3OO=>CH3OOH+R28C5H11 CN	6.0E+0012	0.000	17500.0	! ME 950
C6H12OA-1+R8CH3OO=>CH3OOH+R30C6H11OA 951 CN	6.0E+0012	0.000	20000.0	! ME
C6H12OA-1+R8CH3OO=>CH3OOH+R31C6H11OA 952 CN	3.0E+0012	0.000	17500.0	! ME
C6H12OA-1+R8CH3OO=>CH3OOH+R32C6H11OA 953 CN	3.0E+0012	0.000	17500.0	! ME
C6H12OA-1+R8CH3OO=>CH3OOH+R33C6H11OA 954 CN	3.0E+0012	0.000	17500.0	! ME
C6H12OA-1+R8CH3OO=>CH3OOH+R34C6H11OA 955 CN	3.0E+0012	0.000	17500.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R35C6H11O2K 956	7.6E+0004	2.000	15525.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R36C6H11O2B 957 CN	6.0E+0012	0.000	20000.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R37C6H11O2B 958 CN	3.0E+0012	0.000	17500.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R38C6H11O2B 959 CN	3.0E+0012	0.000	17500.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R39C6H11O2B 960 CN	3.0E+0012	0.000	17500.0	! ME
C6H12O2B-1+R8CH3OO=>CH3OOH+R40C6H11O2B 961 CR	3.0E+0012	0.000	15000.0	! ME
C5H12-1+R11C2H5=>C2H6+R26C5H11	2.0E+0011	0.000	11000.0	! ME 962 CN
C5H12-1+R11C2H5=>C2H6+R27C5H11	6.0E+0011	0.000	13500.0	! ME 963 CR
C5H12-1+R11C2H5=>C2H6+R28C5H11	4.0E+0011	0.000	11000.0	! ME 964 CN
C6H12OA-1+R11C2H5=>C2H6+R30C6H11OA CR	3.0E+0011	0.000	13500.0	! ME 965
C6H12OA-1+R11C2H5=>C2H6+R31C6H11OA CN	2.0E+0011	0.000	11000.0	! ME 966
C6H12OA-1+R11C2H5=>C2H6+R32C6H11OA CN	2.0E+0011	0.000	11000.0	! ME 967
C6H12OA-1+R11C2H5=>C2H6+R33C6H11OA CN	2.0E+0011	0.000	11000.0	! ME 968
C6H12OA-1+R11C2H5=>C2H6+R34C6H11OA CN	2.0E+0011	0.000	11000.0	! ME 969
C6H12O2B-1+R11C2H5=>C2H6+R35C6H11O2K 970	2.3E+0004	2.000	10525.0	! ME
C6H12O2B-1+R11C2H5=>C2H6+R36C6H11O2B 971 CR	3.0E+0011	0.000	13500.0	! ME
C6H12O2B-1+R11C2H5=>C2H6+R37C6H11O2B 972 CN	2.0E+0011	0.000	11000.0	! ME
C6H12O2B-1+R11C2H5=>C2H6+R38C6H11O2B 973 CN	2.0E+0011	0.000	11000.0	! ME

C6H12O2B-1+R11C2H5=>C2H6+R39C6H11O2B 974 CN	2.0E+0011	0.000	11000.0	! ME
C6H12O2B-1+R11C2H5=>C2H6+R40C6H11O2B 975 CR	2.0E+0011	0.000	9200.0	! ME
C5H12-1+R43C5H11O2U=>C5H12O2P+R26C5H11 976 CN	3.0E+0012	0.000	17500.0	! ME
C5H12-1+R43C5H11O2U=>C5H12O2P+R27C5H11 977 CN	1.2E+0013	0.000	20000.0	! ME
C5H12-1+R43C5H11O2U=>C5H12O2P+R28C5H11 978 CN	6.0E+0012	0.000	17500.0	! ME
C6H12OA-1+R43C5H11O2U=>C5H12O2P+R30C6H11OA ! ME 979 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R43C5H11O2U=>C5H12O2P+R31C6H11OA ! ME 980 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R43C5H11O2U=>C5H12O2P+R32C6H11OA ! ME 981 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R43C5H11O2U=>C5H12O2P+R33C6H11OA ! ME 982 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R43C5H11O2U=>C5H12O2P+R34C6H11OA ! ME 983 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R35C6H11O2K ! ME 984	7.6E+0004	2.000	15525.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R36C6H11O2B ! ME 985 CN	6.0E+0012	0.000	20000.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R37C6H11O2B ! ME 986 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R38C6H11O2B ! ME 987 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R39C6H11O2B ! ME 988 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R43C5H11O2U=>C5H12O2P+R40C6H11O2B ! ME 989 CR	3.0E+0012	0.000	15000.0	
C5H12-1+R44C5H11O2U=>C5H12O2P+R26C5H11 990 CN	3.0E+0012	0.000	17500.0	! ME
C5H12-1+R44C5H11O2U=>C5H12O2P+R27C5H11 991 CN	1.2E+0013	0.000	20000.0	! ME
C5H12-1+R44C5H11O2U=>C5H12O2P+R28C5H11 992 CN	6.0E+0012	0.000	17500.0	! ME
C6H12OA-1+R44C5H11O2U=>C5H12O2P+R30C6H11OA ! ME 993 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R44C5H11O2U=>C5H12O2P+R31C6H11OA ! ME 994 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R44C5H11O2U=>C5H12O2P+R32C6H11OA ! ME 995 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R44C5H11O2U=>C5H12O2P+R33C6H11OA ! ME 996 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R44C5H11O2U=>C5H12O2P+R34C6H11OA ! ME 997 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R35C6H11O2K ! ME 998	7.6E+0004	2.000	15525.0	
C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R36C6H11O2B ! ME 999 CN	6.0E+0012	0.000	20000.0	
C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R37C6H11O2B ! ME 1000 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R38C6H11O2B ! ME 1001 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R39C6H11O2B ! ME 1002 CN	3.0E+0012	0.000	17500.0	

C6H12O2B-1+R44C5H11O2U=>C5H12O2P+R40C6H11O2B	3.0E+0012	0.000	15000.0	
! ME 1003 CR				
C5H12-1+R45C5H11O2U=>C5H12O2P+R26C5H11	3.0E+0012	0.000	17500.0	! ME
1004 CN				
C5H12-1+R45C5H11O2U=>C5H12O2P+R27C5H11	1.2E+0013	0.000	20000.0	! ME
1005 CN				
C5H12-1+R45C5H11O2U=>C5H12O2P+R28C5H11	6.0E+0012	0.000	17500.0	! ME
1006 CN				
C6H12OA-1+R45C5H11O2U=>C5H12O2P+R30C6H11OA	6.0E+0012	0.000	20000.0	
! ME 1007 CN				
C6H12OA-1+R45C5H11O2U=>C5H12O2P+R31C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1008 CN				
C6H12OA-1+R45C5H11O2U=>C5H12O2P+R32C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1009 CN				
C6H12OA-1+R45C5H11O2U=>C5H12O2P+R33C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1010 CN				
C6H12OA-1+R45C5H11O2U=>C5H12O2P+R34C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1011 CN				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R35C6H11O2K	7.6E+0004	2.000	15525.0	
! ME 1012				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R36C6H11O2B	6.0E+0012	0.000	20000.0	
! ME 1013 CN				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R37C6H11O2B	3.0E+0012	0.000	17500.0	
! ME 1014 CN				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R38C6H11O2B	3.0E+0012	0.000	17500.0	
! ME 1015 CN				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R39C6H11O2B	3.0E+0012	0.000	17500.0	
! ME 1016 CN				
C6H12O2B-1+R45C5H11O2U=>C5H12O2P+R40C6H11O2B	3.0E+0012	0.000	15000.0	
! ME 1017 CR				
C5H12-1+R46C6H11O3AU=>C6H12O3AP+R26C5H11	3.0E+0012	0.000	17500.0	!
ME 1018 CN				
C5H12-1+R46C6H11O3AU=>C6H12O3AP+R27C5H11	1.2E+0013	0.000	20000.0	!
ME 1019 CN				
C5H12-1+R46C6H11O3AU=>C6H12O3AP+R28C5H11	6.0E+0012	0.000	17500.0	!
ME 1020 CN				
C6H12OA-1+R46C6H11O3AU=>C6H12O3AP+R30C6H11OA	6.0E+0012	0.000	20000.0	
! ME 1021 CN				
C6H12OA-1+R46C6H11O3AU=>C6H12O3AP+R31C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1022 CN				
C6H12OA-1+R46C6H11O3AU=>C6H12O3AP+R32C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1023 CN				
C6H12OA-1+R46C6H11O3AU=>C6H12O3AP+R33C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1024 CN				
C6H12OA-1+R46C6H11O3AU=>C6H12O3AP+R34C6H11OA	3.0E+0012	0.000	17500.0	
! ME 1025 CN				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R35C6H11O2K	7.6E+0004	2.000		
15525.0 ! ME 1026				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R36C6H11O2B	6.0E+0012	0.000		
20000.0 ! ME 1027 CN				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R37C6H11O2B	3.0E+0012	0.000		
17500.0 ! ME 1028 CN				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R38C6H11O2B	3.0E+0012	0.000		
17500.0 ! ME 1029 CN				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R39C6H11O2B	3.0E+0012	0.000		
17500.0 ! ME 1030 CN				
C6H12O2B-1+R46C6H11O3AU=>C6H12O3AP+R40C6H11O2B	3.0E+0012	0.000		
15000.0 ! ME 1031 CR				

C5H12-1+R48C6H11O3AU=>C6H12O3AP+R26C5H11 ME 1032 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R48C6H11O3AU=>C6H12O3AP+R27C5H11 ME 1033 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R48C6H11O3AU=>C6H12O3AP+R28C5H11 ME 1034 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R48C6H11O3AU=>C6H12O3AP+R30C6H11OA ! ME 1035 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R48C6H11O3AU=>C6H12O3AP+R31C6H11OA ! ME 1036 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R48C6H11O3AU=>C6H12O3AP+R32C6H11OA ! ME 1037 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R48C6H11O3AU=>C6H12O3AP+R33C6H11OA ! ME 1038 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R48C6H11O3AU=>C6H12O3AP+R34C6H11OA ! ME 1039 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R35C6H11O2K 15525.0 ! ME 1040	7.6E+0004	2.000		
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R36C6H11O2B 20000.0 ! ME 1041 CN	6.0E+0012	0.000		
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R37C6H11O2B 17500.0 ! ME 1042 CN	3.0E+0012	0.000		
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R38C6H11O2B 17500.0 ! ME 1043 CN	3.0E+0012	0.000		
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R39C6H11O2B 17500.0 ! ME 1044 CN	3.0E+0012	0.000		
C6H12O2B-1+R48C6H11O3AU=>C6H12O3AP+R40C6H11O2B 15000.0 ! ME 1045 CR	3.0E+0012	0.000		
C5H12-1+R50C6H11O3AU=>C6H12O3AP+R26C5H11 ME 1046 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R50C6H11O3AU=>C6H12O3AP+R27C5H11 ME 1047 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R50C6H11O3AU=>C6H12O3AP+R28C5H11 ME 1048 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R50C6H11O3AU=>C6H12O3AP+R30C6H11OA ! ME 1049 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R50C6H11O3AU=>C6H12O3AP+R31C6H11OA ! ME 1050 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R50C6H11O3AU=>C6H12O3AP+R32C6H11OA ! ME 1051 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R50C6H11O3AU=>C6H12O3AP+R33C6H11OA ! ME 1052 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R50C6H11O3AU=>C6H12O3AP+R34C6H11OA ! ME 1053 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R35C6H11O2K 15525.0 ! ME 1054	7.6E+0004	2.000		
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R36C6H11O2B 20000.0 ! ME 1055 CN	6.0E+0012	0.000		
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R37C6H11O2B 17500.0 ! ME 1056 CN	3.0E+0012	0.000		
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R38C6H11O2B 17500.0 ! ME 1057 CN	3.0E+0012	0.000		
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R39C6H11O2B 17500.0 ! ME 1058 CN	3.0E+0012	0.000		
C6H12O2B-1+R50C6H11O3AU=>C6H12O3AP+R40C6H11O2B 15000.0 ! ME 1059 CR	3.0E+0012	0.000		
C5H12-1+R51C6H11O3AU=>C6H12O3AP+R26C5H11 ME 1060 CN	3.0E+0012	0.000	17500.0	!

C5H12-1+R51C6H11O3AU=>C6H12O3AP+R27C5H11 ME 1061 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R51C6H11O3AU=>C6H12O3AP+R28C5H11 ME 1062 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R51C6H11O3AU=>C6H12O3AP+R30C6H11OA ! ME 1063 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R51C6H11O3AU=>C6H12O3AP+R31C6H11OA ! ME 1064 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R51C6H11O3AU=>C6H12O3AP+R32C6H11OA ! ME 1065 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R51C6H11O3AU=>C6H12O3AP+R33C6H11OA ! ME 1066 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R51C6H11O3AU=>C6H12O3AP+R34C6H11OA ! ME 1067 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R35C6H11O2K 15525.0 ! ME 1068	7.6E+0004	2.000		
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R36C6H11O2B 20000.0 ! ME 1069 CN	6.0E+0012	0.000		
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R37C6H11O2B 17500.0 ! ME 1070 CN	3.0E+0012	0.000		
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R38C6H11O2B 17500.0 ! ME 1071 CN	3.0E+0012	0.000		
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R39C6H11O2B 17500.0 ! ME 1072 CN	3.0E+0012	0.000		
C6H12O2B-1+R51C6H11O3AU=>C6H12O3AP+R40C6H11O2B 15000.0 ! ME 1073 CR	3.0E+0012	0.000		
C5H12-1+R52C6H11O3AU=>C6H12O3AP+R26C5H11 ME 1074 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R52C6H11O3AU=>C6H12O3AP+R27C5H11 ME 1075 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R52C6H11O3AU=>C6H12O3AP+R28C5H11 ME 1076 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R52C6H11O3AU=>C6H12O3AP+R30C6H11OA ! ME 1077 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R52C6H11O3AU=>C6H12O3AP+R31C6H11OA ! ME 1078 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R52C6H11O3AU=>C6H12O3AP+R32C6H11OA ! ME 1079 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R52C6H11O3AU=>C6H12O3AP+R33C6H11OA ! ME 1080 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R52C6H11O3AU=>C6H12O3AP+R34C6H11OA ! ME 1081 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R35C6H11O2K 15525.0 ! ME 1082	7.6E+0004	2.000		
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R36C6H11O2B 20000.0 ! ME 1083 CN	6.0E+0012	0.000		
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R37C6H11O2B 17500.0 ! ME 1084 CN	3.0E+0012	0.000		
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R38C6H11O2B 17500.0 ! ME 1085 CN	3.0E+0012	0.000		
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R39C6H11O2B 17500.0 ! ME 1086 CN	3.0E+0012	0.000		
C6H12O2B-1+R52C6H11O3AU=>C6H12O3AP+R40C6H11O2B 15000.0 ! ME 1087 CR	3.0E+0012	0.000		
C5H12-1+R53C6H11O4UB=>C6H12O4PB+R26C5H11 ME 1088 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R53C6H11O4UB=>C6H12O4PB+R27C5H11 ME 1089 CN	1.2E+0013	0.000	20000.0	!

C5H12-1+R53C6H11O4UB=>C6H12O4PB+R28C5H11 ME 1090 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R53C6H11O4UB=>C6H12O4PB+R30C6H11OA ! ME 1091 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R53C6H11O4UB=>C6H12O4PB+R31C6H11OA ! ME 1092 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R53C6H11O4UB=>C6H12O4PB+R32C6H11OA ! ME 1093 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R53C6H11O4UB=>C6H12O4PB+R33C6H11OA ! ME 1094 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R53C6H11O4UB=>C6H12O4PB+R34C6H11OA ! ME 1095 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R35C6H11O2K 15525.0 ! ME 1096	7.6E+0004	2.000		
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R36C6H11O2B 20000.0 ! ME 1097 CN	6.0E+0012	0.000		
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R37C6H11O2B 17500.0 ! ME 1098 CN	3.0E+0012	0.000		
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R38C6H11O2B 17500.0 ! ME 1099 CN	3.0E+0012	0.000		
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R39C6H11O2B 17500.0 ! ME 1100 CN	3.0E+0012	0.000		
C6H12O2B-1+R53C6H11O4UB=>C6H12O4PB+R40C6H11O2B 15000.0 ! ME 1101 CR	3.0E+0012	0.000		
C5H12-1+R55C6H11O4UB=>C6H12O4PB+R26C5H11 ME 1102 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R55C6H11O4UB=>C6H12O4PB+R27C5H11 ME 1103 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R55C6H11O4UB=>C6H12O4PB+R28C5H11 ME 1104 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R55C6H11O4UB=>C6H12O4PB+R30C6H11OA ! ME 1105 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R55C6H11O4UB=>C6H12O4PB+R31C6H11OA ! ME 1106 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R55C6H11O4UB=>C6H12O4PB+R32C6H11OA ! ME 1107 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R55C6H11O4UB=>C6H12O4PB+R33C6H11OA ! ME 1108 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R55C6H11O4UB=>C6H12O4PB+R34C6H11OA ! ME 1109 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R35C6H11O2K 15525.0 ! ME 1110	7.6E+0004	2.000		
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R36C6H11O2B 20000.0 ! ME 1111 CN	6.0E+0012	0.000		
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R37C6H11O2B 17500.0 ! ME 1112 CN	3.0E+0012	0.000		
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R38C6H11O2B 17500.0 ! ME 1113 CN	3.0E+0012	0.000		
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R39C6H11O2B 17500.0 ! ME 1114 CN	3.0E+0012	0.000		
C6H12O2B-1+R55C6H11O4UB=>C6H12O4PB+R40C6H11O2B 15000.0 ! ME 1115 CR	3.0E+0012	0.000		
C5H12-1+R57C6H11O4UB=>C6H12O4PB+R26C5H11 ME 1116 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R57C6H11O4UB=>C6H12O4PB+R27C5H11 ME 1117 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R57C6H11O4UB=>C6H12O4PB+R28C5H11 ME 1118 CN	6.0E+0012	0.000	17500.0	!

C6H12OA-1+R57C6H11O4UB=>C6H12O4PB+R30C6H11OA ! ME 1119 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R57C6H11O4UB=>C6H12O4PB+R31C6H11OA ! ME 1120 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R57C6H11O4UB=>C6H12O4PB+R32C6H11OA ! ME 1121 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R57C6H11O4UB=>C6H12O4PB+R33C6H11OA ! ME 1122 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R57C6H11O4UB=>C6H12O4PB+R34C6H11OA ! ME 1123 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R35C6H11O2K 15525.0 ! ME 1124	7.6E+0004	2.000		
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R36C6H11O2B 20000.0 ! ME 1125 CN	6.0E+0012	0.000		
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R37C6H11O2B 17500.0 ! ME 1126 CN	3.0E+0012	0.000		
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R38C6H11O2B 17500.0 ! ME 1127 CN	3.0E+0012	0.000		
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R39C6H11O2B 17500.0 ! ME 1128 CN	3.0E+0012	0.000		
C6H12O2B-1+R57C6H11O4UB=>C6H12O4PB+R40C6H11O2B 15000.0 ! ME 1129 CR	3.0E+0012	0.000		
C5H12-1+R58C6H11O4UB=>C6H12O4PB+R26C5H11 ME 1130 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R58C6H11O4UB=>C6H12O4PB+R27C5H11 ME 1131 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R58C6H11O4UB=>C6H12O4PB+R28C5H11 ME 1132 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R58C6H11O4UB=>C6H12O4PB+R30C6H11OA ! ME 1133 CN	6.0E+0012	0.000	20000.0	
C6H12OA-1+R58C6H11O4UB=>C6H12O4PB+R31C6H11OA ! ME 1134 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R58C6H11O4UB=>C6H12O4PB+R32C6H11OA ! ME 1135 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R58C6H11O4UB=>C6H12O4PB+R33C6H11OA ! ME 1136 CN	3.0E+0012	0.000	17500.0	
C6H12OA-1+R58C6H11O4UB=>C6H12O4PB+R34C6H11OA ! ME 1137 CN	3.0E+0012	0.000	17500.0	
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R35C6H11O2K 15525.0 ! ME 1138	7.6E+0004	2.000		
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R36C6H11O2B 20000.0 ! ME 1139 CN	6.0E+0012	0.000		
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R37C6H11O2B 17500.0 ! ME 1140 CN	3.0E+0012	0.000		
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R38C6H11O2B 17500.0 ! ME 1141 CN	3.0E+0012	0.000		
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R39C6H11O2B 17500.0 ! ME 1142 CN	3.0E+0012	0.000		
C6H12O2B-1+R58C6H11O4UB=>C6H12O4PB+R40C6H11O2B 15000.0 ! ME 1143 CR	3.0E+0012	0.000		
C5H12-1+R59C6H11O4UB=>C6H12O4PB+R26C5H11 ME 1144 CN	3.0E+0012	0.000	17500.0	!
C5H12-1+R59C6H11O4UB=>C6H12O4PB+R27C5H11 ME 1145 CN	1.2E+0013	0.000	20000.0	!
C5H12-1+R59C6H11O4UB=>C6H12O4PB+R28C5H11 ME 1146 CN	6.0E+0012	0.000	17500.0	!
C6H12OA-1+R59C6H11O4UB=>C6H12O4PB+R30C6H11OA ! ME 1147 CN	6.0E+0012	0.000	20000.0	



C6H12OA-1+R59C6H11O4UB=>C6H12O4PB+R31C6H11OA 3.0E+0012 0.000 17500.0  
 ! ME 1148 CN  
 C6H12OA-1+R59C6H11O4UB=>C6H12O4PB+R32C6H11OA 3.0E+0012 0.000 17500.0  
 ! ME 1149 CN  
 C6H12OA-1+R59C6H11O4UB=>C6H12O4PB+R33C6H11OA 3.0E+0012 0.000 17500.0  
 ! ME 1150 CN  
 C6H12OA-1+R59C6H11O4UB=>C6H12O4PB+R34C6H11OA 3.0E+0012 0.000 17500.0  
 ! ME 1151 CN  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R35C6H11O2K 7.6E+0004 2.000  
 15525.0 ! ME 1152  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R36C6H11O2B 6.0E+0012 0.000  
 20000.0 ! ME 1153 CN  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R37C6H11O2B 3.0E+0012 0.000  
 17500.0 ! ME 1154 CN  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R38C6H11O2B 3.0E+0012 0.000  
 17500.0 ! ME 1155 CN  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R39C6H11O2B 3.0E+0012 0.000  
 17500.0 ! ME 1156 CN  
 C6H12O2B-1+R59C6H11O4UB=>C6H12O4PB+R40C6H11O2B 3.0E+0012 0.000  
 15000.0 ! ME 1157 CR  
 C5H12-1+R229C3H7=>C3H8+R26C5H11 2.8E-0003 4.200 8000.0 ! ME 1158 CN  
 C5H12-1+R229C3H7=>C3H8+R27C5H11 8.4E-0003 4.200 8700.0 ! ME 1159 CN  
 C5H12-1+R229C3H7=>C3H8+R28C5H11 5.6E-0003 4.200 8000.0 ! ME 1160 CN  
 C6H12OA-1+R229C3H7=>C3H8+R30C6H11OA 4.2E-0003 4.200 8700.0 ! ME  
 1161 CN  
 C6H12OA-1+R229C3H7=>C3H8+R31C6H11OA 2.8E-0003 4.200 8000.0 ! ME  
 1162 CN  
 C6H12OA-1+R229C3H7=>C3H8+R32C6H11OA 2.8E-0003 4.200 8000.0 ! ME  
 1163 CN  
 C6H12OA-1+R229C3H7=>C3H8+R33C6H11OA 2.8E-0003 4.200 8000.0 ! ME  
 1164 CN  
 C6H12OA-1+R229C3H7=>C3H8+R34C6H11OA 2.8E-0003 4.200 8000.0 ! ME  
 1165 CN  
 C6H12O2B-1+R229C3H7=>C3H8+R35C6H11O2K 1.4E+0004 2.000 11525.0 ! ME  
 1166  
 C6H12O2B-1+R229C3H7=>C3H8+R36C6H11O2B 4.2E-0003 4.200 8700.0 ! ME  
 1167 CN  
 C6H12O2B-1+R229C3H7=>C3H8+R37C6H11O2B 2.8E-0003 4.200 8000.0 ! ME  
 1168 CN  
 C6H12O2B-1+R229C3H7=>C3H8+R38C6H11O2B 2.8E-0003 4.200 8000.0 ! ME  
 1169 CN  
 C6H12O2B-1+R229C3H7=>C3H8+R39C6H11O2B 2.8E-0003 4.200 8000.0 ! ME  
 1170 CN  
 C6H12O2B-1+R229C3H7=>C3H8+R40C6H11O2B 2.8E-0003 4.200 6000.0 ! ME  
 1171 CR

! combinations :

R1H+R229C3H7=>C3H8 8.3E+0015 0.000 0.0 ! CO 1172 KB  
 R2OH+R229C3H7=>C3H8OL 5.9E+0015 0.000 0.0 ! CO 1173 KB  
 R3OOH+R229C3H7=>C3H8O2P 4.8E+0015 0.000 0.0 ! CO 1174 KB  
 R4CH3+R229C3H7=>C4H10 1.5E+0016 0.000 0.0 ! CO 1175 KB  
 R5CHO+R229C3H7=>C4H8OA 5.2E+0015 0.000 0.0 ! CO 1176 KB  
 R6CH2OH+R229C3H7=>C4H10OL 5.1E+0015 0.000 0.0 ! CO 1177 KB  
 R11C2H5+R229C3H7=>M102C5H12 5.2E+0015 0.000 0.0 ! CO 1178 KB  
 R229C3H7+R229C3H7=>C6H14 2.3E+0015 0.000 0.0 ! CO 1179 KB

! dismutations :

R41C3H7O2U+R3OOH=>C3H8O2P+O2 2.0E+0011 0.000 -1300.0 ! DI 1180 CN

R42C4H9O2U+R3OOH=>C4H10O2P+O2	2.0E+0011	0.000	-1300.0	!	DI 1181	CN
R43C5H11O2U+R3OOH=>C5H12O2P+O2	2.0E+0011	0.000	-1300.0	!	DI 1182	CN
R44C5H11O2U+R3OOH=>C5H12O2P+O2	2.0E+0011	0.000	-1300.0	!	DI 1183	CN
R45C5H11O2U+R3OOH=>C5H12O2P+O2	2.0E+0011	0.000	-1300.0	!	DI 1184	CN
R46C6H11O3AU+R3OOH=>C6H12O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1185	CN
R48C6H11O3AU+R3OOH=>C6H12O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1186	CN
R50C6H11O3AU+R3OOH=>C6H12O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1187	CN
R51C6H11O3AU+R3OOH=>C6H12O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1188	CN
R52C6H11O3AU+R3OOH=>C6H12O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1189	CN
R53C6H11O4UB+R3OOH=>C6H12O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1190	CN
R55C6H11O4UB+R3OOH=>C6H12O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1191	CN
R57C6H11O4UB+R3OOH=>C6H12O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1192	CN
R58C6H11O4UB+R3OOH=>C6H12O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1193	CN
R59C6H11O4UB+R3OOH=>C6H12O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1194	CN
R79C4H7O3AU+R3OOH=>C4H8O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1195	CN
R86C3H5O3AU+R3OOH=>C3H6O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1196	CN
R106C4H7O4UB+R3OOH=>C4H8O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1197	CN
R111C3H5O4UB+R3OOH=>C3H6O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1198	CN
R203C3H7O2U+R3OOH=>C3H8O2P+O2	2.0E+0011	0.000	-1300.0	!	DI 1199	CN
R210C4H7O3AU+R3OOH=>C4H8O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1200	CN
R214C3H5O3AU+R3OOH=>C3H6O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1201	CN
R216C4H7O3AU+R3OOH=>C4H8O3AP+O2	2.0E+0011	0.000	-1300.0	!	DI 1202	CN
R224C4H7O4UB+R3OOH=>C4H8O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1203	CN
R226C3H5O4UB+R3OOH=>C3H6O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1204	CN
R228C4H7O4UB+R3OOH=>C4H8O4PB+O2	2.0E+0011	0.000	-1300.0	!	DI 1205	CN

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

! Peroxide decomposition

! Hydroperoxide decomposition

!C5H12O2P=>R2OH+R19C3H7+CH3CHO	1.5E+0016	0.000	43000.0	!	DHP 1206
C5H12O2P=>R2OH+R11C2H5+C2H5CHO	1.5E+0016	0.000	43000.0	!	
C3H6O2PZ=>R2OH+R1H+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP 1207
C4H8O2PZ=>R2OH+R4CH3+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP 1208
C5H10O2PZ=>R2OH+R11C2H5+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP 1209
C3H8O2P=>R2OH+R11C2H5+HCHO	1.5E+0016	0.000	43000.0	!	DHP 1210
C4H10O2P=>R2OH+R11C2H5+CH3CHO	1.5E+0016	0.000	43000.0	!	DHP 1211

C3H6O2PY=>R2OH+R1H+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 1212  
C4H8O2PY=>R2OH+R4CH3+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 1213  
C5H10O2PY=>R2OH+R11C2H5+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 1214

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

C3H6O3KP=>B2CO+R2OH+R4CH3+HCHO 1.5E+0016 0.000 43000.0 ! DKP 1215  
C4H8O3KP=>B2CO+R2OH+R11C2H5+HCHO 1.5E+0016 0.000 43000.0 ! DKP 1216  
C5H10O3KP=>B2CO+R2OH+R11C2H5+CH3CHO 1.5E+0016 0.000 43000.0 ! DKP  
1217  
C6H10O3KPZ=>R2OH+R5CHO+B2CO+2C2H4Z 1.5E+0016 0.000 43000.0 ! KPZ  
1218  
C4H6O3KPZ=>R2OH+R5CHO+B2CO+C2H4Z 1.5E+0016 0.000 43000.0 ! KPZ 1219  
C3H4O3KPZ=>R2OH+R13CH2CHO+B2CO 1.5E+0016 0.000 43000.0 ! KPZ 1220

! Aldohydroperoxide decomposition

!C6H12O3AP=>R2OH+CH3CHO+C2H4Z+R13CH2CHO 1.5E+0016 0.000 43000.0 !  
DAP 1221

!Olive

C6H12O3AP=>R2OH+C6H11OKO 1.5E+0016 0.000 43000.0 !

!

C5H8O3APZ=>R2OH+CH2COZ+C2H4Z+R5CHO 1.5E+0016 0.000 43000.0 ! DAP  
1222

C4H6O3APZ=>R2OH+CH2COZ+R13CH2CHO 1.5E+0016 0.000 43000.0 ! DAP 1223

C3H4O3APZ=>R2OH+CH2COZ+R5CHO 1.5E+0016 0.000 43000.0 ! DAP 1224

C4H8O3AP=>R2OH+CH3CHO+R13CH2CHO 1.5E+0016 0.000 43000.0 ! DAP 1225

C3H6O3AP=>R2OH+CH3CHO+R5CHO 1.5E+0016 0.000 43000.0 ! DAP 1226

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions

C3H8+R1H=>H2+R19C3H7 5.7E+0007 2.000 7700.0 ! MH 1227

DUPLICATE

C3H8+R1H=>H2+R19C3H7 9.0E+0006 2.000 5000.0 ! MH 1228

DUPLICATE

C3H8+R2OH=>H2O+R19C3H7 1.3E+0006 2.000 -765.0 ! MH 1229

DUPLICATE

C3H8+R2OH=>H2O+R19C3H7 9.0E+0006 2.000 5000.0 ! MH 1230

DUPLICATE

C3H8+R3OOH=>H2O2+R19C3H7 1.2E+0012 0.000 17000.0 ! MH 1231

DUPLICATE

C3H8+R3OOH=>H2O2+R19C3H7 4.0E+0011 0.000 15500.0 ! MH 1232

DUPLICATE

C3H8+R4CH3=>CH4+R19C3H7 6.0E-0001 4.000 8200.0 ! MH 1233

DUPLICATE

C3H8+R4CH3=>CH4+R19C3H7 2.0E+0011 0.000 9600.0 ! MH 1234

DUPLICATE

C3H8+R8CH3OO=>CH3OOH+R19C3H7 1.2E+0013 0.000 20000.0 ! MH 1235

DUPLICATE

C3H8+R8CH3OO=>CH3OOH+R19C3H7	3.0E+0012	0.000	17500.0	! MH 1236
DUPLICATE				
C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	! MH 1237
DUPLICATE				
C3H8+R11C2H5=>C2H6+R19C3H7	2.0E+0011	0.000	11000.0	! MH 1238
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	5.7E+0007	2.000	7700.0	! MH 1239
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	1.8E+0007	2.000	5000.0	! MH 1240
DUPLICATE				
C4H10+R2OH=>H2O+R20C4H9	1.3E+0006	2.000	-765.0	! MH 1241
DUPLICATE				
C4H10+R2OH=>H2O+R20C4H9	1.8E+0007	2.000	5000.0	! MH 1242
DUPLICATE				
C4H10+R3OOH=>H2O2+R20C4H9	1.2E+0012	0.000	17000.0	! MH 1243
DUPLICATE				
C4H10+R3OOH=>H2O2+R20C4H9	8.0E+0011	0.000	15500.0	! MH 1244
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	6.0E-0001	4.000	8200.0	! MH 1245
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	4.0E+0011	0.000	9600.0	! MH 1246
DUPLICATE				
C4H10+R8CH3OO=>CH3OOH+R20C4H9	1.2E+0013	0.000	20000.0	! MH 1247
DUPLICATE				
C4H10+R8CH3OO=>CH3OOH+R20C4H9	6.0E+0012	0.000	17500.0	! MH 1248
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	6.0E+0011	0.000	13500.0	! MH 1249
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	4.0E+0011	0.000	11000.0	! MH 1250
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	5.7E+0007	2.000	7700.0	! MH 1251
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	1.8E+0007	2.000	5000.0	! MH 1252
DUPLICATE				
C4H10+R2OH=>H2O+R20C4H9	1.3E+0006	2.000	-765.0	! MH 1253
DUPLICATE				
C4H10+R2OH=>H2O+R20C4H9	1.8E+0007	2.000	5000.0	! MH 1254
DUPLICATE				
C4H10+R3OOH=>H2O2+R20C4H9	1.2E+0012	0.000	17000.0	! MH 1255
DUPLICATE				
C4H10+R3OOH=>H2O2+R20C4H9	8.0E+0011	0.000	15500.0	! MH 1256
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	6.0E-0001	4.000	8200.0	! MH 1257
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	4.0E+0011	0.000	9600.0	! MH 1258
DUPLICATE				
C4H10+R8CH3OO=>CH3OOH+R20C4H9	1.2E+0013	0.000	20000.0	! MH 1259
DUPLICATE				
C4H10+R8CH3OO=>CH3OOH+R20C4H9	6.0E+0012	0.000	17500.0	! MH 1260
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	6.0E+0011	0.000	13500.0	! MH 1261
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	4.0E+0011	0.000	11000.0	! MH 1262
DUPLICATE				
!C5H12+R1H=>H2+R26C5H11	5.7E+0007	2.000	7700.0	! MH 1263
! DUPLICATE				
!C5H12+R1H=>H2+R26C5H11	2.7E+0007	2.000	5000.0	! MH 1264
! DUPLICATE				

!C5H12+R2OH=>H2O+R26C5H11	1.3E+0006	2.000	-765.0	! MH 1265
! DUPLICATE				
!C5H12+R2OH=>H2O+R26C5H11	2.7E+0007	2.000	5000.0	! MH 1266
! DUPLICATE				
!C5H12+R3OOH=>H2O2+R26C5H11	1.2E+0012	0.000	17000.0	! MH 1267
! DUPLICATE				
!C5H12+R3OOH=>H2O2+R26C5H11	1.2E+0012	0.000	15500.0	! MH 1268
! DUPLICATE				
!C5H12+R4CH3=>CH4+R26C5H11	6.0E-0001	4.000	8200.0	! MH 1269
! DUPLICATE				
!C5H12+R4CH3=>CH4+R26C5H11	6.0E+0011	0.000	9600.0	! MH 1270
! DUPLICATE				
!C5H12+R8CH3OO=>CH3OOH+R26C5H11	1.2E+0013	0.000	20000.0	! MH 1271
! DUPLICATE				
!C5H12+R8CH3OO=>CH3OOH+R26C5H11	9.0E+0012	0.000	17500.0	! MH 1272
! DUPLICATE				
!C5H12+R11C2H5=>C2H6+R26C5H11	6.0E+0011	0.000	13500.0	! MH 1273
! DUPLICATE				
!C5H12+R11C2H5=>C2H6+R26C5H11	6.0E+0011	0.000	11000.0	! MH 1274
! DUPLICATE				
C6H14+R1H=>H2+R11C2H5+2C2H4Z	5.7E+0007	2.000	7700.0	! MH 1275
DUPLICATE				
C6H14+R1H=>H2+R11C2H5+2C2H4Z	3.6E+0007	2.000	5000.0	! MH 1276
DUPLICATE				
C6H14+R2OH=>H2O+R11C2H5+2C2H4Z	5.4E+0006	2.000	450.0	! MH 1277
DUPLICATE				
C6H14+R2OH=>H2O+R11C2H5+2C2H4Z	1.0E+0007	2.000	-765.0	! MH 1278
DUPLICATE				
C6H14+R3OOH=>H2O2+R11C2H5+2C2H4Z	1.2E+0012	0.000	17000.0	! MH 1279
DUPLICATE				
C6H14+R3OOH=>H2O2+R11C2H5+2C2H4Z	1.6E+0012	0.000	15500.0	! MH 1280
DUPLICATE				
C6H14+R4CH3=>CH4+R11C2H5+2C2H4Z	6.0E-0001	4.000	8200.0	! MH 1281
DUPLICATE				
C6H14+R4CH3=>CH4+R11C2H5+2C2H4Z	8.0E+0011	0.000	9600.0	! MH 1282
DUPLICATE				
C6H14+R8CH3OO=>CH3OOH+R11C2H5+2C2H4Z	1.5E+0012	0.000	17500.0	! MH 1283
DUPLICATE				
C6H14+R8CH3OO=>CH3OOH+R11C2H5+2C2H4Z	5.3E-0306	0.000	0.0	! MH 1284
DUPLICATE				
C6H14+R11C2H5=>C2H6+R11C2H5+2C2H4Z	1.0E+0011	0.000	11000.0	! MH 1285
DUPLICATE				
C6H14+R11C2H5=>C2H6+R11C2H5+2C2H4Z	5.3E-0306	0.000	0.0	! MH 1286
DUPLICATE				
! O-ring decomposition				
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ	2.9E+0007	2.000	7700.0	! DEu 1287
DUPLICATE				
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ	1.3E+0007	2.000	5000.0	! DEi 1288
DUPLICATE				
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ	2.7E+0006	2.000	450.0	! DEu 1289
DUPLICATE				
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ	3.9E+0006	2.000	-765.0	! DEi 1290
DUPLICATE				
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ	6.0E+0011	0.000	17000.0	! DEu 1291

DUPLICATE  
 C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ 6.0E+0011 0.000 15500.0 ! DEi  
 1292  
 DUPLICATE  
 C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ 3.0E-0001 4.000 8200.0 ! DEu 1293  
 DUPLICATE  
 C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ 3.0E+0011 0.000 9600.0 ! DEi 1294  
 DUPLICATE  
 C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ 6.0E+0012 0.000 20000.0 ! DEu  
 1295  
 DUPLICATE  
 C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ 4.5E+0012 0.000 17500.0 ! DEi  
 1296  
 DUPLICATE  
 C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ 3.0E+0011 0.000 13500.0 ! DEu  
 1297  
 DUPLICATE  
 C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ 3.0E+0011 0.000 11000.0 ! DEi  
 1298  
 DUPLICATE  
 C3H6OE#4+R1H=>H2+R4CH3+CH2COZ 2.7E+0007 2.000 5000.0 ! DEu 1299  
 C3H6OE#4+R2OH=>H2O+R4CH3+CH2COZ 7.8E+0006 2.000 -765.0 ! DEu 1300  
 C3H6OE#4+R3OOH=>H2O2+R4CH3+CH2COZ 1.2E+0012 0.000 15500.0 ! DEu  
 1301  
 C3H6OE#4+R4CH3=>CH4+R4CH3+CH2COZ 6.0E+0011 0.000 9600.0 ! DEu 1302  
 C3H6OE#4+R8CH3OO=>CH3OOH+R4CH3+CH2COZ 9.0E+0012 0.000 17500.0 ! DEu  
 1303  
 C3H6OE#4+R11C2H5=>C2H6+R4CH3+CH2COZ 6.0E+0011 0.000 11000.0 ! DEu  
 1304  
 C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ 2.9E+0007 2.000 7700.0 ! DEu 1305  
 DUPLICATE  
 C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ 2.3E+0007 2.000 5000.0 ! DEi 1306  
 DUPLICATE  
 C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ 2.7E+0006 2.000 450.0 ! DEu 1307  
 DUPLICATE  
 C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ 6.5E+0006 2.000 -765.0 ! DEi 1308  
 DUPLICATE  
 C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ 6.0E+0011 0.000 17000.0 ! DEu  
 1309  
 DUPLICATE  
 C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ 1.0E+0012 0.000 15500.0 ! DEi  
 1310  
 DUPLICATE  
 C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ 3.0E-0001 4.000 8200.0 ! DEu  
 1311  
 DUPLICATE  
 C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ 5.0E+0011 0.000 9600.0 ! DEi  
 1312  
 DUPLICATE  
 C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ 6.0E+0012 0.000 20000.0 !  
 DEu 1313  
 DUPLICATE  
 C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ 7.5E+0012 0.000 17500.0 !  
 DEi 1314  
 DUPLICATE  
 C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ 3.0E+0011 0.000 13500.0 ! DEu  
 1315  
 DUPLICATE

C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ 5.0E+0011 0.000 11000.0 ! DEi  
 1316  
 DUPLICATE  
 C4H8OE#4+R1H=>H2+R11C2H5+CH2COZ 2.9E+0007 2.000 7700.0 ! DEu 1317  
 DUPLICATE  
 C4H8OE#4+R1H=>H2+R11C2H5+CH2COZ 2.3E+0007 2.000 5000.0 ! DEi 1318  
 DUPLICATE  
 C4H8OE#4+R2OH=>H2O+R11C2H5+CH2COZ 2.7E+0006 2.000 450.0 ! DEu 1319  
 DUPLICATE  
 C4H8OE#4+R2OH=>H2O+R11C2H5+CH2COZ 6.5E+0006 2.000 -765.0 ! DEi 1320  
 DUPLICATE  
 C4H8OE#4+R3OOH=>H2O2+R11C2H5+CH2COZ 6.0E+0011 0.000 17000.0 ! DEu  
 1321  
 DUPLICATE  
 C4H8OE#4+R3OOH=>H2O2+R11C2H5+CH2COZ 1.0E+0012 0.000 15500.0 ! DEi  
 1322  
 DUPLICATE  
 C4H8OE#4+R4CH3=>CH4+R11C2H5+CH2COZ 3.0E-0001 4.000 8200.0 ! DEu  
 1323  
 DUPLICATE  
 C4H8OE#4+R4CH3=>CH4+R11C2H5+CH2COZ 5.0E+0011 0.000 9600.0 ! DEi  
 1324  
 DUPLICATE  
 C4H8OE#4+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ 6.0E+0012 0.000 20000.0 !  
 DEu 1325  
 DUPLICATE  
 C4H8OE#4+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ 7.5E+0012 0.000 17500.0 !  
 DEi 1326  
 DUPLICATE  
 C4H8OE#4+R11C2H5=>C2H6+R11C2H5+CH2COZ 3.0E+0011 0.000 13500.0 ! DEu  
 1327  
 DUPLICATE  
 C4H8OE#4+R11C2H5=>C2H6+R11C2H5+CH2COZ 5.0E+0011 0.000 11000.0 ! DEi  
 1328  
 DUPLICATE  
 C4H8OE#5+R1H=>H2+R11C2H5+CH2COZ 3.6E+0007 2.000 5000.0 ! DEu 1329  
 C4H8OE#5+R2OH=>H2O+R11C2H5+CH2COZ 1.0E+0007 2.000 -765.0 ! DEu 1330  
 C4H8OE#5+R3OOH=>H2O2+R11C2H5+CH2COZ 1.6E+0012 0.000 15500.0 ! DEu  
 1331  
 C4H8OE#5+R4CH3=>CH4+R11C2H5+CH2COZ 8.0E+0011 0.000 9600.0 ! DEu  
 1332  
 C4H8OE#5+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ 1.2E+0013 0.000 17500.0 !  
 DEu 1333  
 C4H8OE#5+R11C2H5=>C2H6+R11C2H5+CH2COZ 8.0E+0011 0.000 11000.0 ! DEu  
 1334  
 M9C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ 2.9E+0007 2.000 7700.0 ! DEr  
 1335  
 DUPLICATE  
 M9C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ 3.2E+0007 2.000 5000.0 ! DEt  
 1336  
 DUPLICATE  
 M7C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ 2.9E+0007 2.000 7700.0 ! DEr  
 1337  
 DUPLICATE  
 M7C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ 3.2E+0007 2.000 5000.0 ! DEt  
 1338  
 DUPLICATE

M9C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ 1339	2.7E+0006	2.000	450.0	! DEr
DUPLICATE				
M9C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ 1340	9.1E+0006	2.000	-765.0	! DEt
DUPLICATE				
M7C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ 1341	2.7E+0006	2.000	450.0	! DEr
DUPLICATE				
M7C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ 1342	9.1E+0006	2.000	-765.0	! DEt
DUPLICATE				
M9C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ DEr 1343	6.0E+0011	0.000	17000.0	!
DUPLICATE				
M9C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ DEt 1344	1.4E+0012	0.000	15500.0	!
DUPLICATE				
M7C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ DEr 1345	6.0E+0011	0.000	17000.0	!
DUPLICATE				
M7C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ DEt 1346	1.4E+0012	0.000	15500.0	!
DUPLICATE				
M9C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ 1347	3.0E-0001	4.000	8200.0	! DEr
DUPLICATE				
M9C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ 1348	7.0E+0011	0.000	9600.0	! DEt
DUPLICATE				
M7C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ 1349	3.0E-0001	4.000	8200.0	! DEr
DUPLICATE				
M7C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ 1350	7.0E+0011	0.000	9600.0	! DEt
DUPLICATE				
M9C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ ! DEr 1351	6.0E+0012	0.000	20000.0	
DUPLICATE				
M9C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ ! DEt 1352	1.0E+0013	0.000	17500.0	
DUPLICATE				
M7C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ ! DEr 1353	6.0E+0012	0.000	20000.0	
DUPLICATE				
M7C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ ! DEt 1354	1.0E+0013	0.000	17500.0	
DUPLICATE				
M9C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ DEr 1355	3.0E+0011	0.000	13500.0	!
DUPLICATE				
M9C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ DEt 1356	7.0E+0011	0.000	11000.0	!
DUPLICATE				
M7C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ DEr 1357	3.0E+0011	0.000	13500.0	!
DUPLICATE				



M7C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ 7.0E+0011 0.000 11000.0 !  
DEt 1358  
DUPLICATE  
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ 2.9E+0007 2.000 7700.0 ! DEu  
1359  
DUPLICATE  
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ 4.1E+0007 2.000 5000.0 ! DEi  
1360  
DUPLICATE  
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ 2.7E+0006 2.000 450.0 ! DEu  
1361  
DUPLICATE  
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ 1.1E+0007 2.000 -765.0 ! DEi  
1362  
DUPLICATE  
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ 6.0E+0011 0.000 17000.0 !  
DEu 1363  
DUPLICATE  
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ 1.8E+0012 0.000 15500.0 !  
DEi 1364  
DUPLICATE  
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 3.0E-0001 4.000 8200.0 ! DEu  
1365  
DUPLICATE  
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 9.0E+0011 0.000 9600.0 ! DEi  
1366  
DUPLICATE  
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ 6.0E+0012 0.000 20000.0  
! DEu 1367  
DUPLICATE  
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ 1.3E+0013 0.000 17500.0  
! DEi 1368  
DUPLICATE  
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ 3.0E+0011 0.000 13500.0 !  
DEu 1369  
DUPLICATE  
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ 9.0E+0011 0.000 11000.0 !  
DEi 1370  
DUPLICATE  
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ 2.9E+0007 2.000 7700.0 ! DEu  
1371  
DUPLICATE  
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ 5.0E+0007 2.000 5000.0 ! DEi  
1372  
DUPLICATE  
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ 2.7E+0006 2.000 450.0 ! DEu  
1373  
DUPLICATE  
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ 1.4E+0007 2.000 -765.0 ! DEi  
1374  
DUPLICATE  
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ 6.0E+0011 0.000 17000.0 !  
DEu 1375  
DUPLICATE  
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ 2.2E+0012 0.000 15500.0 !  
DEi 1376  
DUPLICATE

C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ 3.0E-0001 4.000 8200.0 ! DEu  
 1377  
 DUPLICATE  
 C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ 1.1E+0012 0.000 9600.0 ! DEi  
 1378  
 DUPLICATE  
 C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ 6.0E+0012 0.000 20000.0  
 ! DEu 1379  
 DUPLICATE  
 C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ 1.7E+0013 0.000 17500.0  
 ! DEi 1380  
 DUPLICATE  
 C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ 3.0E+0011 0.000 13500.0 !  
 DEu 1381  
 DUPLICATE  
 C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ 1.1E+0012 0.000 11000.0 !  
 DEi 1382  
 DUPLICATE  
 C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ 2.9E+0007 2.000 7700.0 ! DEu 1383  
 DUPLICATE  
 C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ 5.9E+0007 2.000 5000.0 ! DEi 1384  
 DUPLICATE  
 C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ 2.7E+0006 2.000 450.0 ! DEu  
 1385  
 DUPLICATE  
 C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ 1.7E+0007 2.000 -765.0 ! DEi  
 1386  
 DUPLICATE  
 C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ 6.0E+0011 0.000 17000.0 ! DEu  
 1387  
 DUPLICATE  
 C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ 2.6E+0012 0.000 15500.0 ! DEi  
 1388  
 DUPLICATE  
 C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ 3.0E-0001 4.000 8200.0 ! DEu  
 1389  
 DUPLICATE  
 C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ 1.3E+0012 0.000 9600.0 ! DEi  
 1390  
 DUPLICATE  
 C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ 6.0E+0012 0.000 20000.0 !  
 DEu 1391  
 DUPLICATE  
 C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ 2.0E+0013 0.000 17500.0 !  
 DEi 1392  
 DUPLICATE  
 C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ 3.0E+0011 0.000 13500.0 !  
 DEu 1393  
 DUPLICATE  
 C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ 1.3E+0012 0.000 11000.0 !  
 DEi 1394  
 DUPLICATE

! Metatheses of oxetanes, furanes and pyranes

M12C5H10OE#4+R1H=>H2+C5H9OE#4 2.9E+0007 2.000 7700.0 ! ME# 1395  
 DUPLICATE  
 M12C5H10OE#4+R1H=>H2+C5H9OE#4 3.2E+0007 2.000 5000.0 ! ME# 1396

DUPLICATE  
 M8C5H10OE#4+R1H=>H2+C5H9OE#4 2.9E+0007 2.000 7700.0 ! ME# 1397  
 DUPLICATE  
 M8C5H10OE#4+R1H=>H2+C5H9OE#4 3.2E+0007 2.000 5000.0 ! ME# 1398  
 DUPLICATE  
 M12C5H10OE#4+R2OH=>H2O+C5H9OE#4 2.7E+0006 2.000 450.0 ! ME# 1399  
 DUPLICATE  
 M12C5H10OE#4+R2OH=>H2O+C5H9OE#4 9.1E+0006 2.000 -765.0 ! ME# 1400  
 DUPLICATE  
 M8C5H10OE#4+R2OH=>H2O+C5H9OE#4 2.7E+0006 2.000 450.0 ! ME# 1401  
 DUPLICATE  
 M8C5H10OE#4+R2OH=>H2O+C5H9OE#4 9.1E+0006 2.000 -765.0 ! ME# 1402  
 DUPLICATE  
 M12C5H10OE#4+R3OOH=>H2O2+C5H9OE#4 6.0E+0011 0.000 17000.0 ! ME#  
 1403  
 DUPLICATE  
 M12C5H10OE#4+R3OOH=>H2O2+C5H9OE#4 1.4E+0012 0.000 15500.0 ! ME#  
 1404  
 DUPLICATE  
 M8C5H10OE#4+R3OOH=>H2O2+C5H9OE#4 6.0E+0011 0.000 17000.0 ! ME# 1405  
 DUPLICATE  
 M8C5H10OE#4+R3OOH=>H2O2+C5H9OE#4 1.4E+0012 0.000 15500.0 ! ME# 1406  
 DUPLICATE  
 M12C5H10OE#4+R4CH3=>CH4+C5H9OE#4 3.0E-0001 4.000 8200.0 ! ME# 1407  
 DUPLICATE  
 M12C5H10OE#4+R4CH3=>CH4+C5H9OE#4 7.0E+0011 0.000 9600.0 ! ME# 1408  
 DUPLICATE  
 M8C5H10OE#4+R4CH3=>CH4+C5H9OE#4 3.0E-0001 4.000 8200.0 ! ME# 1409  
 DUPLICATE  
 M8C5H10OE#4+R4CH3=>CH4+C5H9OE#4 7.0E+0011 0.000 9600.0 ! ME# 1410  
 DUPLICATE  
 M12C5H10OE#4+R8CH3OO=>CH3OOH+C5H9OE#4 6.0E+0012 0.000 20000.0 ! ME#  
 1411  
 DUPLICATE  
 M12C5H10OE#4+R8CH3OO=>CH3OOH+C5H9OE#4 1.0E+0013 0.000 17500.0 ! ME#  
 1412  
 DUPLICATE  
 M8C5H10OE#4+R8CH3OO=>CH3OOH+C5H9OE#4 6.0E+0012 0.000 20000.0 ! ME#  
 1413  
 DUPLICATE  
 M8C5H10OE#4+R8CH3OO=>CH3OOH+C5H9OE#4 1.0E+0013 0.000 17500.0 ! ME#  
 1414  
 DUPLICATE  
 M12C5H10OE#4+R11C2H5=>C2H6+C5H9OE#4 3.0E+0011 0.000 13500.0 ! ME#  
 1415  
 DUPLICATE  
 M12C5H10OE#4+R11C2H5=>C2H6+C5H9OE#4 7.0E+0011 0.000 11000.0 ! ME#  
 1416  
 DUPLICATE  
 M8C5H10OE#4+R11C2H5=>C2H6+C5H9OE#4 3.0E+0011 0.000 13500.0 ! ME#  
 1417  
 DUPLICATE  
 M8C5H10OE#4+R11C2H5=>C2H6+C5H9OE#4 7.0E+0011 0.000 11000.0 ! ME#  
 1418  
 DUPLICATE  
 !2-methyl-THF  
 M10C5H10OE#5+R1H=>H2+C5H9OE#5 2.9E+0007 2.000 7700.0 ! ME# 1419  
 DUPLICATE

M10C5H10OE#5+R1H=>H2+C5H9OE#5 2.7E+0007 2.000 5000.0 ! ME# 1420  
DUPLICATE  
M10C5H10OE#5+R1H=>H2+C5H9OE#5 4.2E+0006 2.000 2400.0 ! added by  
Olivier  
DUPLICATE  
M10C5H10OE#5+R2OH=>H2O+C5H9OE#5 2.7E+0006 2.000 450.0 ! ME# 1421  
DUPLICATE  
M10C5H10OE#5+R2OH=>H2O+C5H9OE#5 7.8E+0006 2.000 -765.0 ! ME# 1422  
DUPLICATE  
M10C5H10OE#5+R2OH=>H2O+C5H9OE#5 1.1E+0006 2.000 -1870.0 ! added by  
Olivier  
DUPLICATE  
M10C5H10OE#5+R3OOH=>H2O2+C5H9OE#5 6.0E+0011 0.000 17000.0 ! ME#  
1423  
DUPLICATE  
M10C5H10OE#5+R3OOH=>H2O2+C5H9OE#5 1.2E+0012 0.000 15500.0 ! ME#  
1424  
DUPLICATE  
M10C5H10OE#5+R3OOH=>H2O2+C5H9OE#5 1.0E+0012 0.000 14000.0 ! added  
by Olivier  
DUPLICATE  
M10C5H10OE#5+R4CH3=>CH4+C5H9OE#5 3.0E-0001 4.000 8200.0 ! ME# 1425  
DUPLICATE  
M10C5H10OE#5+R4CH3=>CH4+C5H9OE#5 6.0E+0011 0.000 9600.0 ! ME# 1426  
DUPLICATE  
M10C5H10OE#5+R4CH3=>CH4+C5H9OE#5 1.0E+0011 0.000 7900.0 ! added by  
Olivier  
DUPLICATE  
M10C5H10OE#5+R8CH3OO=>CH3OOH+C5H9OE#5 6.0E+0012 0.000 20000.0 ! ME#  
1427  
DUPLICATE  
M10C5H10OE#5+R8CH3OO=>CH3OOH+C5H9OE#5 9.0E+0012 0.000 17500.0 ! ME#  
1428  
DUPLICATE  
M10C5H10OE#5+R8CH3OO=>CH3OOH+C5H9OE#5 1.5E+0012 0.000 15000.0 !  
added by Olivier  
DUPLICATE  
M10C5H10OE#5+R11C2H5=>C2H6+C5H9OE#5 3.0E+0011 0.000 13500.0 ! ME#  
1429  
DUPLICATE  
M10C5H10OE#5+R11C2H5=>C2H6+C5H9OE#5 6.0E+0011 0.000 11000.0 ! ME#  
1430  
DUPLICATE  
M10C5H10OE#5+R11C2H5=>C2H6+C5H9OE#5 1.0E+0011 0.000 9200.0 ! added  
by Olivier  
DUPLICATE  
M11C5H10OE#6+R1H=>H2+C5H9OE#6 4.5E+0007 2.000 5000.0 ! ME# 1431  
M11C5H10OE#6+R2OH=>H2O+C5H9OE#6 1.3E+0007 2.000 -765.0 ! ME# 1432  
M11C5H10OE#6+R3OOH=>H2O2+C5H9OE#6 2.0E+0012 0.000 15500.0 ! ME#  
1433  
M11C5H10OE#6+R4CH3=>CH4+C5H9OE#6 1.0E+0012 0.000 9600.0 ! ME# 1434  
M11C5H10OE#6+R8CH3OO=>CH3OOH+C5H9OE#6 1.5E+0013 0.000 17500.0 ! ME#  
1435  
M11C5H10OE#6+R11C2H5=>C2H6+C5H9OE#6 1.0E+0012 0.000 11000.0 ! ME#  
1436  
!  
! Metatheses of capro-lactones  
!gcaprolac

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gcaprolac+R1H=>H2+C2H4Z+B2CO+C2H4Z+R5CHO      2.9E+0007  2.000  7700.0  !
added by Olivier
gcaprolac+R1H=>H2+CO2+C2H4Z+RC3H5Y      1.8E+0007  2.000  5000.0  ! added
by Olivier
gcaprolac+R1H=>H2+B2CO+B2CO+C2H4Z+R11C2H5      4.2E+0006  2.000  2400.0  !
added by Olivier
gcaprolac+R2OH=>H2O+C2H4Z+B2CO+C2H4Z+R5CHO      2.7E+0006  2.000  450.0  !
added by Olivier
gcaprolac+R2OH=>H2O+CO2+C2H4Z+RC3H5Y      5.2E+0006  2.000  -765.0  ! added
by Olivier
gcaprolac+R2OH=>H2O+B2CO+B2CO+C2H4Z+R11C2H5      1.1E+0006  2.000  -1870.0
! added by Olivier
gcaprolac+R3OOH=>H2O2+C2H4Z+B2CO+C2H4Z+R5CHO      6.0E+0011  0.000  17000.0
! added by Olivier
gcaprolac+R3OOH=>H2O2+CO2+C2H4Z+RC3H5Y      0.8E+0012  0.000  15500.0  !
added by Olivier
gcaprolac+R3OOH=>H2O2+B2CO+B2CO+C2H4Z+R11C2H5      1.0E+0012  0.000
14000.0  ! added by Olivier
gcaprolac+R4CH3=>CH4+C2H4Z+B2CO+C2H4Z+R5CHO      3.0E-0001  4.000  8200.0
! added by Olivier
gcaprolac+R4CH3=>CH4+CO2+C2H4Z+RC3H5Y      4.0E+0011  0.000  9600.0  !
added by Olivier
gcaprolac+R4CH3=>CH4+B2CO+B2CO+C2H4Z+R11C2H5      1.0E+0011  0.000  7900.0
! added by Olivier
gcaprolac+R8CH3OO=>CH3OOH+C2H4Z+B2CO+C2H4Z+R5CHO      6.0E+0012  0.000
20000.0  ! added by Olivier
gcaprolac+R8CH3OO=>CH3OOH+CO2+C2H4Z+RC3H5Y      6.0E+0012  0.000  17500.0
! added by Olivier
gcaprolac+R8CH3OO=>CH3OOH+B2CO+B2CO+C2H4Z+R11C2H5      1.5E+0012  0.000
15000.0  ! added by Olivier
gcaprolac+R11C2H5=>C2H6+C2H4Z+B2CO+C2H4Z+R5CHO      3.0E+0011  0.000
13500.0  ! added by Olivier
gcaprolac+R11C2H5=>C2H6+CO2+C2H4Z+RC3H5Y      4.0E+0011  0.000  11000.0  !
added by Olivier
gcaprolac+R11C2H5=>C2H6+B2CO+B2CO+C2H4Z+R11C2H5      1.0E+0011  0.000
9200.0  ! added by Olivier
!dcaprolac
dcaprolac+R1H=>H2+CO2+C2H4Z+RC3H5Y      3.6E+0007  2.000  5000.0  ! added
by Olivier
dcaprolac+R2OH=>H2O+CO2+C2H4Z+RC3H5Y      1.04E+0007  2.000  -765.0  !
added by Olivier
dcaprolac+R3OOH=>H2O2+CO2+C2H4Z+RC3H5Y      1.6E+0012  0.000  15500.0  !
added by Olivier
dcaprolac+R4CH3=>CH4+CO2+C2H4Z+RC3H5Y      0.8E+0012  0.000  9600.0  !
added by Olivier
dcaprolac+R8CH3OO=>CH3OOH+CO2+C2H4Z+RC3H5Y      1.2E+0013  0.000  17500.0
! added by Olivier
dcaprolac+R11C2H5=>C2H6+CO2+C2H4Z+RC3H5Y      0.8E+0012  0.000  11000.0  !
added by Olivier

! decompositions of cyclo-ether radicals
C5H9OE#4=>R13CH2CHO+C3H6Z      5.0E+0013  0.000  24800.0  ! DEm 1437
C5H9OE#5=>R13CH2CHO+C3H6Z      5.0E+0013  0.000  24800.0  ! DEm 1438
C5H9OE#6=>R13CH2CHO+C3H6Z      5.0E+0013  0.000  24800.0  ! DEm 1439

! Addition of oxygen on cyclo-ether radicals
C5H9OE#4+O2=>C5H9O3E#4U      3.0E+0019  -2.500  0.0  ! ??? 1440
C5H9OE#5+O2=>C5H9O3E#5U      3.0E+0019  -2.500  0.0  ! ??? 1441

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C5H9OE#6+O2=>C5H9O3E#6U 3.0E+0019 -2.500 0.0 ! ??? 1442  
 C5H9O3E#4U=>C5H9OE#4+O2 5.0E+0022 -2.500 40000.0 ! ??? 1443  
 C5H9O3E#5U=>C5H9OE#5+O2 5.0E+0022 -2.500 40000.0 ! ??? 1444  
 C5H9O3E#6U=>C5H9OE#6+O2 5.0E+0022 -2.500 40000.0 ! ??? 1445  
 ! O2 elimination  
 ! Isomerization  
 ! Cylo-ether keto-hydroperoxide ester formation  
 ! Decomposition of cylo-ether keto-hydroperoxide ester  
  
 ! Isomerization of peroxy-radicals  
 C5H9O3E#4U=>C5H9O3E#4P 8.0E+0013 0.000 25500.0 ! ??? 1446  
 C5H9O3E#5U=>C5H9O3E#5P 8.0E+0013 0.000 25500.0 ! ??? 1447  
 C5H9O3E#6U=>C5H9O3E#6P 8.0E+0013 0.000 25500.0 ! ??? 1448  
 C5H9O3E#4P=>C5H9O3E#4U 4.8E+0012 0.000 19000.0 ! ??? 1449  
 C5H9O3E#5P=>C5H9O3E#5U 4.8E+0012 0.000 19000.0 ! ??? 1450  
 C5H9O3E#6P=>C5H9O3E#6U 4.8E+0012 0.000 19000.0 ! ??? 1451  
  
 !Addition of oxygen on cyclo-peroxy radicals  
 C5H9O3E#4P+O2=>C5H9O5E#4UP 3.0E+0019 -2.500 0.0 ! ??? 1452  
 C5H9O3E#5P+O2=>C5H9O5E#5UP 3.0E+0019 -2.500 0.0 ! ??? 1453  
 C5H9O3E#6P+O2=>C5H9O5E#6UP 3.0E+0019 -2.500 0.0 ! ??? 1454  
 C5H9O5E#4UP=>C5H9O3E#4P+O2 5.0E+0022 -2.500 40000.0 ! ??? 1455  
 C5H9O5E#5UP=>C5H9O3E#5P+O2 5.0E+0022 -2.500 40000.0 ! ??? 1456  
 C5H9O5E#6UP=>C5H9O3E#6P+O2 5.0E+0022 -2.500 40000.0 ! ??? 1457  
  
 ! Formation of cyclo-ether ketohydroperoxydes  
 C5H9O5E#4UP=>R2OH+C5H8O4E#4KP 1.0E+0009 0.000 7500.0 ! ??? 1458  
 C5H9O5E#5UP=>R2OH+C5H8O4E#5KP 1.0E+0009 0.000 7500.0 ! ??? 1459  
 C5H9O5E#6UP=>R2OH+C5H8O4E#6KP 1.0E+0009 0.000 7500.0 ! ??? 1460  
  
 ! Decomposition of cyclo-ether ketohydroperoxydes  
 C5H8O4E#4KP=>R2OH+CO2+R5CHO+C3H6Z 1.5E+0016 0.000 43000.0 ! #KP  
 1461  
 C5H8O4E#5KP=>R2OH+CO2+R5CHO+C3H6Z 1.5E+0016 0.000 43000.0 ! #KP  
 1462  
 C5H8O4E#6KP=>R2OH+CO2+R5CHO+C3H6Z 1.5E+0016 0.000 43000.0 ! #KP  
 1463  
  
 ! Olefin reactions  
 ! addition of H and CH3 on olefins  
 C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 1560.0 ! \*7 1464  
 DUPLICATE  
 C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 3260.0 ! \*8 1465  
 DUPLICATE  
 nC4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 1560.0 ! \*7 1466  
 DUPLICATE  
 nC4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 3260.0 ! \*8 1467  
 DUPLICATE  
 nC4H8Y+R4CH3=>C3H6Y+R11C2H5 9.6E+0010 0.000 8000.0 ! \*7 1468  
 M31C5H10Y+R1H=>R26C5H11 1.3E+0013 0.000 1560.0 ! \*5 1469  
 DUPLICATE  
 M31C5H10Y+R1H=> R26C5H11 1.3E+0013 0.000 3260.0 ! \*6 1470  
 DUPLICATE  
 M31C5H10Y+R4CH3=>nC4H8Y+R11C2H5 1.7E+0011 0.000 7400.0 ! \*5 1471  
 M31C5H10Y+R4CH3=>C3H6Y+R19C3H7 9.6E+0010 0.000 8000.0 ! \*5 1472  
 M32C5H10Z+R1H=>R26C5H11 1.3E+0013 0.000 1560.0 ! \*5 1473  
 DUPLICATE  
 M32C5H10Z+R1H=> R26C5H11 1.3E+0013 0.000 3260.0 ! \*6 1474

DUPLICATE  
 M32C5H10Z+R4CH3=>nC4H8Y+R11C2H5 1.7E+0011 0.000 7400.0 ! \*5 1475  
 M32C5H10Z+R4CH3=>C3H6Y+R19C3H7 9.6E+0010 0.000 8000.0 ! \*5 1476  
 C4H8Z+R1H=>R20C4H9 1.3E+0013 0.000 1560.0 ! \*9 1477  
 DUPLICATE  
 C4H8Z+R1H=>R20C4H9 1.3E+0013 0.000 3260.0 ! \*10 1478  
 DUPLICATE  
 C4H8Z+R4CH3=>C3H6Y+R11C2H5 9.6E+0010 0.000 8000.0 ! \*9 1479  
 C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 1560.0 ! \*9 1480  
 DUPLICATE  
 C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 3260.0 ! \*10 1481  
 DUPLICATE  
 C4H8Y+R4CH3=>C3H6Y+R11C2H5 9.6E+0010 0.000 8000.0 ! \*9 1482  
 C6H12Z+R4CH3=>nC4H8Y+R19C3H7 1.7E+0011 0.000 7400.0 ! \*9 1483  
 C6H12Z+R4CH3=>C3H6Y+R20C4H9 9.6E+0010 0.000 8000.0 ! \*9 1484  
 C7H14Z+R4CH3=>nC4H8Y+R20C4H9 1.7E+0011 0.000 7400.0 ! \*9 1485  
 C7H14Z+R4CH3=>C3H6Y+R26C5H11 9.6E+0010 0.000 8000.0 ! \*9 1486  
 C8H16Z+R4CH3=>nC4H8Y+R26C5H11 1.7E+0011 0.000 7400.0 ! \*9 1487  
 C6H12Z+R1H=>2C2H4Z+R11C2H5 9.6E+0010 0.000 8000.0 ! \*13 1488  
 C7H14Z+R1H=>3C2H4Z+R4CH3 9.6E+0010 0.000 8000.0 ! \*13 1489  
 C8H16Z+R1H=>3C2H4Z+R11C2H5 9.6E+0010 0.000 8000.0 ! \*13 1490  
  
 ! addition of OH on olefins  
 C3H6Y+R2OH=>R4CH3+CH3CHO 1.4E+0012 0.000 -1040.0 ! \*16 1491  
 C3H6Y+R2OH=>R11C2H5+HCHO 1.4E+0012 0.000 -1040.0 ! \*16 1492  
 nC4H8Y+R2OH=>R4CH3+C2H5CHO 1.4E+0012 0.000 -1040.0 ! \*16 1493  
 nC4H8Y+R2OH=>R19C3H7+HCHO 1.4E+0012 0.000 -1040.0 ! \*16 1494  
 M31C5H10Y+R2OH=>R4CH3+C4H8OA 1.4E+0012 0.000 -1040.0 ! \*15 1495  
 M31C5H10Y+R2OH=>R20C4H9+HCHO 1.4E+0012 0.000 -1040.0 ! \*15 1496  
 M32C5H10Z+R2OH=>R4CH3+C4H8OA 1.4E+0012 0.000 -1040.0 ! \*15 1497  
 M32C5H10Z+R2OH=>R20C4H9+HCHO 1.4E+0012 0.000 -1040.0 ! \*15 1498  
 C4H8Z+R2OH=>R4CH3+C2H5CHO 1.4E+0012 0.000 -1040.0 ! \*17 1499  
 C4H8Z+R2OH=>R19C3H7+HCHO 1.4E+0012 0.000 -1040.0 ! \*17 1500  
 C4H8Y+R2OH=>R4CH3+C2H5CHO 1.4E+0012 0.000 -1040.0 ! \*17 1501  
 C4H8Y+R2OH=>R19C3H7+HCHO 1.4E+0012 0.000 -1040.0 ! \*17 1502  
 C6H12Z+R2OH=>R4CH3+C5H10OA 1.4E+0012 0.000 -1040.0 ! \*17 1503  
 C6H12Z+R2OH=>R26C5H11+HCHO 1.4E+0012 0.000 -1040.0 ! \*17 1504  
 C7H14Z+R2OH=>R4CH3+C6H12OA 1.4E+0012 0.000 -1040.0 ! \*17 1505  
 C8H16Z+R2OH=>R4CH3+C7H14OA 1.4E+0012 0.000 -1040.0 ! \*17 1506  
  
 C7H14Z+R2OH=>HCHO+R11C2H5+2C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 1507  
 C8H16Z+R2OH=>HCHO+R4CH3+3C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 1508  
  
 ! addition of O on olefins  
 C3H6Y+B1O=>CH2COZ+R1H+R4CH3 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 nC4H8Y+B1O=>CH2COZ+R1H+R11C2H5 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 M31C5H10Y+B1O=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ  
 1509  
 M32C5H10Z+B1O=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ  
 1509  
 C4H8Z+B1O=>CH2COZ+R1H+R11C2H5 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 C4H8Y+B1O=>CH2COZ+R1H+R11C2H5 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 C6H12Z+B1O=>CH2COZ+R1H+R20C4H9 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 C7H14Z+B1O=>CH2COZ+R1H+R26C5H11 1.2E+0005 2.560 -1130.0 ! AOZ 1509  
 C8H16Z+B1O=>CH2COZ+R11C2H5+R1H+2C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ  
 1509  
  
 ! retroene reactions

M31C5H10Y=>C3H6Y+C2H4Z	8.0E+0012	0.000	56500.0	! RTZ 1509
M32C5H10Z=>C3H6Y+C2H4Z	8.0E+0012	0.000	56500.0	! RTZ 1510
C6H12Z=>C3H6Y+C3H6Y	8.0E+0012	0.000	56500.0	! RTZ 1511
C7H14Z=>C3H6Y+C4H8Z	8.0E+0012	0.000	56500.0	! RTZ 1512
C8H16Z=>C3H6Y+M32C5H10Z	8.0E+0012	0.000	56500.0	! RTZ 1513
! addition of OOH on olefins				
C3H6Y+R3OOH=>R2OH+C3H6OE#3	1.0E+0012	0.000	14200.0	! *32 1514
nC4H8Y+R3OOH=>R2OH+C4H8OE#3	1.0E+0012	0.000	14200.0	! *32 1515
M31C5H10Y+R3OOH=>R2OH+M9C5H10OE#3	5.2E+0011	0.000	14200.0	! *28 1516
M31C5H10Y+R3OOH=>R2OH+M7C5H10OE#3	5.2E+0011	0.000	14200.0	! *28 1517
M32C5H10Z+R3OOH=>R2OH+M9C5H10OE#3	5.2E+0011	0.000	14200.0	! *28 1518
M32C5H10Z+R3OOH=>R2OH+M7C5H10OE#3	5.2E+0011	0.000	14200.0	! *28 1519
C4H8Z+R3OOH=>R2OH+C4H8OE#3	1.0E+0012	0.000	14200.0	! *34 1520
C4H8Y+R3OOH=>R2OH+C4H8OE#3	1.0E+0012	0.000	14200.0	! *34 1521
C6H12Z+R3OOH=>R2OH+C6H12OE#3	1.0E+0012	0.000	14200.0	! *34 1522
C7H14Z+R3OOH=>R2OH+C7H14OE#3	1.0E+0012	0.000	14200.0	! *34 1523
C8H16Z+R3OOH=>R2OH+C8H16OE#3	1.0E+0012	0.000	14200.0	! *34 1524
! olefin to dienes				
M32C5H10Z+R1H=>H2+C4H6Z2+R4CH3	5.4E+0004	2.500	-1900.0	! MZ 1525
DUPLICATE				
M32C5H10Z+R1H=>H2+C4H6Z2+R4CH3	2.9E+0007	2.000	7700.0	! MZ 1526
DUPLICATE				
M32C5H10Z+R1H=>H2+C4H6Z2+R4CH3	9.0E+0006	2.000	5000.0	! MZ 1527
DUPLICATE				
M32C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3	3.0E+0006	2.000	-1520.0	! MZ 1528
DUPLICATE				
M32C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3	2.7E+0006	2.000	450.0	! MZ 1529
DUPLICATE				
M32C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3	2.6E+0006	2.000	-765.0	! MZ 1530
DUPLICATE				
M32C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3	6.4E+0003	2.600	12400.0	! MZ 1531
DUPLICATE				
M32C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3	6.0E+0011	0.000	17000.0	! MZ 1532
DUPLICATE				
M32C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3	4.0E+0011	0.000	15500.0	! MZ 1533
DUPLICATE				
M32C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	1.0E+0011	0.000	7300.0	! MZ 1534
DUPLICATE				
M32C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	3.0E-0001	4.000	8200.0	! MZ 1535
DUPLICATE				
M32C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	2.0E+0011	0.000	9600.0	! MZ 1536
DUPLICATE				
M32C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3	1.0E+0012	0.000	14550.0	! MZ 1537
DUPLICATE				
M32C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3	6.0E+0012	0.000	20000.0	! MZ 1538
DUPLICATE				



M32C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3 1539	3.0E+0012	0.000	17500.0	! MZ
DUPLICATE				
M32C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3 1540	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
M32C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3 1541	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
M32C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3 1542	2.0E+0011	0.000	11000.0	! MZ
DUPLICATE				
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 1543
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 1544
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	1.8E+0007	2.000	5000.0	! MZ 1545
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 1546
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 1547
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5 DUPLICATE	5.2E+0006	2.000	-765.0	! MZ 1548
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 1549
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 1550
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	8.0E+0011	0.000	15500.0	! MZ 1551
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 1552
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 1553
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	4.0E+0011	0.000	9600.0	! MZ 1554
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5 1555	1.0E+0012	0.000	14550.0	! MZ
DUPLICATE				
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5 1556	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5 1557	6.0E+0012	0.000	17500.0	! MZ
DUPLICATE				
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 1558	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 1559	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 1560	4.0E+0011	0.000	11000.0	! MZ
DUPLICATE				
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 1561
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 1562

C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	2.7E+0007	2.000	5000.0	! MZ 1563
DUPLICATE				
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7	3.0E+0006	2.000	-1520.0	! MZ 1564
DUPLICATE				
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7	2.7E+0006	2.000	450.0	! MZ 1565
DUPLICATE				
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7	7.8E+0006	2.000	-765.0	! MZ 1566
DUPLICATE				
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7	6.4E+0003	2.600	12400.0	! MZ 1567
DUPLICATE				
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7	6.0E+0011	0.000	17000.0	! MZ 1568
DUPLICATE				
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7	1.2E+0012	0.000	15500.0	! MZ 1569
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	1.0E+0011	0.000	7300.0	! MZ 1570
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	3.0E-0001	4.000	8200.0	! MZ 1571
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	6.0E+0011	0.000	9600.0	! MZ 1572
DUPLICATE				
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7	1.0E+0012	0.000	14550.0	! MZ 1573
DUPLICATE				
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7	6.0E+0012	0.000	20000.0	! MZ 1574
DUPLICATE				
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7	9.0E+0012	0.000	17500.0	! MZ 1575
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	1.5E+0000	3.500	4140.0	! MZ 1576
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	3.0E+0011	0.000	13500.0	! MZ 1577
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	6.0E+0011	0.000	11000.0	! MZ 1578
DUPLICATE				
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	5.4E+0004	2.500	-1900.0	! MZ 1579
DUPLICATE				
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	2.9E+0007	2.000	7700.0	! MZ 1580
DUPLICATE				
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	3.6E+0007	2.000	5000.0	! MZ 1581
DUPLICATE				
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9	3.0E+0006	2.000	-1520.0	! MZ 1582
DUPLICATE				
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9	2.7E+0006	2.000	450.0	! MZ 1583
DUPLICATE				
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9	1.0E+0007	2.000	-765.0	! MZ 1584
DUPLICATE				
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9	6.4E+0003	2.600	12400.0	! MZ 1585
DUPLICATE				
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9	6.0E+0011	0.000	17000.0	! MZ 1586
DUPLICATE				
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9	1.6E+0012	0.000	15500.0	! MZ 1587
DUPLICATE				
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9	1.0E+0011	0.000	7300.0	! MZ 1588
DUPLICATE				

C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 3.0E-0001 4.000 8200.0 ! MZ 1589  
 DUPLICATE  
 C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 8.0E+0011 0.000 9600.0 ! MZ 1590  
 DUPLICATE  
 C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 1.0E+0012 0.000 14550.0 ! MZ  
 1591  
 DUPLICATE  
 C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 6.0E+0012 0.000 20000.0 ! MZ  
 1592  
 DUPLICATE  
 C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 1.2E+0013 0.000 17500.0 ! MZ  
 1593  
 DUPLICATE  
 C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 1.5E+0000 3.500 4140.0 ! MZ  
 1594  
 DUPLICATE  
 C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 3.0E+0011 0.000 13500.0 ! MZ  
 1595  
 DUPLICATE  
 C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 8.0E+0011 0.000 11000.0 ! MZ  
 1596  
 DUPLICATE  
 M32C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3 8.8E+0010 0.700 3250.0 ! MZ 1597  
 DUPLICATE  
 M32C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3 5.1E+0013 0.000 7850.0 ! MZ 1598  
 DUPLICATE  
 M32C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3 2.6E+0013 0.000 5200.0 ! MZ 1599  
 DUPLICATE  
 C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5 8.8E+0010 0.700 3250.0 ! MZ 1600  
 DUPLICATE  
 C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5 5.1E+0013 0.000 7850.0 ! MZ 1601  
 DUPLICATE  
 C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5 5.2E+0013 0.000 5200.0 ! MZ 1602  
 DUPLICATE  
 C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7 8.8E+0010 0.700 3250.0 ! MZ 1603  
 DUPLICATE  
 C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7 5.1E+0013 0.000 7850.0 ! MZ 1604  
 DUPLICATE  
 C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7 7.8E+0013 0.000 5200.0 ! MZ 1605  
 DUPLICATE  
 C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9 8.8E+0010 0.700 3250.0 ! MZ 1606  
 DUPLICATE  
 C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9 5.1E+0013 0.000 7850.0 ! MZ 1607  
 DUPLICATE  
 C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9 1.0E+0014 0.000 5200.0 ! MZ 1608  
 DUPLICATE

! Metathesis with YH

C3H6Y+R1H=>RC3H5Y+H2 1.7E+0005 2.500 2510.0 ! MES 1609  
 C3H6Y+R2OH=>RC3H5Y+H2O 3.0E+0006 2.000 -298.0 ! MES 1610  
 C3H6Y+R3OOH=>RC3H5Y+H2O2 9.6E+0003 2.600 13900.0 ! MES 1611  
 C3H6Y+R4CH3=>RC3H5Y+CH4 2.2E+0000 3.500 5670.0 ! MES 1612  
 C3H6Y+R8CH300=>RC3H5Y+CH300H 2.0E+0012 0.000 17050.0 ! MES 1613  
 C3H6Y+R11C2H5=>RC3H5Y+C2H6 2.2E+0000 3.500 6640.0 ! MES 1614  
 nC4H8Y+R1H=>RC4H7Y+H2 5.4E+0004 2.500 -1900.0 ! MES 1615  
 DUPLICATE  
 nC4H8Y+R1H=>RC4H7Y+H2 2.9E+0007 2.000 7700.0 ! MES 1616  
 DUPLICATE

nC4H8Y+R2OH=>RC4H7Y+H2O	3.0E+0006	2.000	-1520.0	! MES 1617
DUPLICATE				
nC4H8Y+R2OH=>RC4H7Y+H2O	2.7E+0006	2.000	450.0	! MES 1618
DUPLICATE				
nC4H8Y+R3OOH=>RC4H7Y+H2O2	6.4E+0003	2.600	12400.0	! MES 1619
DUPLICATE				
nC4H8Y+R3OOH=>RC4H7Y+H2O2	6.0E+0011	0.000	17000.0	! MES 1620
DUPLICATE				
nC4H8Y+R4CH3=>RC4H7Y+CH4	1.0E+0011	0.000	7300.0	! MES 1621
DUPLICATE				
nC4H8Y+R4CH3=>RC4H7Y+CH4	3.0E-0001	4.000	8200.0	! MES 1622
DUPLICATE				
nC4H8Y+R8CH3OO=>RC4H7Y+CH3OOH	1.0E+0012	0.000	14550.0	! MES 1623
DUPLICATE				
nC4H8Y+R8CH3OO=>RC4H7Y+CH3OOH	6.0E+0012	0.000	20000.0	! MES 1624
DUPLICATE				
nC4H8Y+R11C2H5=>RC4H7Y+C2H6	1.5E+0000	3.500	4140.0	! MES 1625
DUPLICATE				
nC4H8Y+R11C2H5=>RC4H7Y+C2H6	3.0E+0011	0.000	13500.0	! MES 1626
DUPLICATE				
M31C5H10Y+R1H=>RC5H9Y+H2	5.4E+0004	2.500	-1900.0	! MES 1627
DUPLICATE				
M31C5H10Y+R1H=>RC5H9Y+H2	2.9E+0007	2.000	7700.0	! MES 1628
DUPLICATE				
M31C5H10Y+R1H=>RC5H9Y+H2	9.0E+0006	2.000	5000.0	! MES 1629
DUPLICATE				
M31C5H10Y+R2OH=>RC5H9Y+H2O	3.0E+0006	2.000	-1520.0	! MES 1630
DUPLICATE				
M31C5H10Y+R2OH=>RC5H9Y+H2O	2.7E+0006	2.000	450.0	! MES 1631
DUPLICATE				
M31C5H10Y+R2OH=>RC5H9Y+H2O	2.6E+0006	2.000	-765.0	! MES 1632
DUPLICATE				
M31C5H10Y+R3OOH=>RC5H9Y+H2O2	6.4E+0003	2.600	12400.0	! MES 1633
DUPLICATE				
M31C5H10Y+R3OOH=>RC5H9Y+H2O2	6.0E+0011	0.000	17000.0	! MES 1634
DUPLICATE				
M31C5H10Y+R3OOH=>RC5H9Y+H2O2	4.0E+0011	0.000	15500.0	! MES 1635
DUPLICATE				
M31C5H10Y+R4CH3=>RC5H9Y+CH4	1.0E+0011	0.000	7300.0	! MES 1636
DUPLICATE				
M31C5H10Y+R4CH3=>RC5H9Y+CH4	3.0E-0001	4.000	8200.0	! MES 1637
DUPLICATE				
M31C5H10Y+R4CH3=>RC5H9Y+CH4	2.0E+0011	0.000	9600.0	! MES 1638
DUPLICATE				
M31C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH	1.0E+0012	0.000	14550.0	! MES 1639
DUPLICATE				
M31C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH	6.0E+0012	0.000	20000.0	! MES 1640
DUPLICATE				
M31C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH	3.0E+0012	0.000	17500.0	! MES 1641
DUPLICATE				
M31C5H10Y+R11C2H5=>RC5H9Y+C2H6	1.5E+0000	3.500	4140.0	! MES 1642
DUPLICATE				
M31C5H10Y+R11C2H5=>RC5H9Y+C2H6	3.0E+0011	0.000	13500.0	! MES 1643
DUPLICATE				
M31C5H10Y+R11C2H5=>RC5H9Y+C2H6	2.0E+0011	0.000	11000.0	! MES 1644
DUPLICATE				
C4H8Y+R1H=>RC4H7Y+H2	5.4E+0004	2.500	-1900.0	! MES 1645
C4H8Y+R2OH=>RC4H7Y+H2O	3.0E+0006	2.000	-1520.0	! MES 1646

C4H8Y+R3OOH=>RC4H7Y+H2O2 6.4E+0003 2.600 12400.0 ! MES 1647  
C4H8Y+R4CH3=>RC4H7Y+CH4 1.0E+0011 0.000 7300.0 ! MES 1648  
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH 1.0E+0012 0.000 14550.0 ! MES 1649  
C4H8Y+R11C2H5=>RC4H7Y+C2H6 1.5E+0000 3.500 4140.0 ! MES 1650  
C3H6Y+B1O=>RC3H5Y+R2OH 1.7E+0011 0.700 5900.0 ! MES 1651  
nC4H8Y+B1O=>RC4H7Y+R2OH 8.8E+0010 0.700 3250.0 ! MES 1652  
DUPLICATE  
nC4H8Y+B1O=>RC4H7Y+R2OH 5.1E+0013 0.000 7850.0 ! MES 1653  
DUPLICATE  
M31C5H10Y+B1O=>RC5H9Y+R2OH 8.8E+0010 0.700 3250.0 ! MES 1654  
DUPLICATE  
M31C5H10Y+B1O=>RC5H9Y+R2OH 5.1E+0013 0.000 7850.0 ! MES 1655  
DUPLICATE  
M31C5H10Y+B1O=>RC5H9Y+R2OH 2.6E+0013 0.000 5200.0 ! MKZ 1656  
DUPLICATE  
C4H8Y+B1O=>RC4H7Y+R2OH 8.8E+0010 0.700 3250.0 ! MES 1657

! Addition of .Y on YH  
RC3H5Y+M31C5H10Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 1658  
RC3H5Y+nC4H8Y=>R10C2H3V+M32C5H10Z 6.0E+0009 0.000 11400.0 ! ADY 1659  
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Z 6.0E+0009 0.000 11400.0 ! ADY 1660  
RC4H7Y+M31C5H10Y=>R10C2H3V+C7H14Z 6.0E+0009 0.000 11400.0 ! ADY 1661  
RC4H7Y+nC4H8Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 1662  
RC4H7Y+C3H6Y=>R10C2H3V+M32C5H10Z 6.0E+0009 0.000 11400.0 ! ADY 1663  
RC5H9Y+M31C5H10Y=>R10C2H3V+C8H16Z 6.0E+0009 0.000 11400.0 ! ADY 1664  
RC5H9Y+nC4H8Y=>R10C2H3V+C7H14Z 6.0E+0009 0.000 11400.0 ! ADY 1665  
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 1666

! Alcohol reactions  
C3H7OH+R1H=>H2+R2OH+C3H6Y 2.9E+0007 2.000 7700.0 ! MOL 1667  
DUPLICATE  
C3H7OH+R1H=>H2+R2OH+C3H6Y 1.8E+0007 2.000 5000.0 ! MOL 1668  
DUPLICATE  
C3H7OH+R1H=>H2+R11C2H5+HCHO 2.4E+0006 2.000 6525.0 ! MOL 1669  
C3H7OH+R2OH=>H2O+R2OH+C3H6Y 2.7E+0006 2.000 450.0 ! MOL 1670  
DUPLICATE  
C3H7OH+R2OH=>H2O+R2OH+C3H6Y 5.2E+0006 2.000 -765.0 ! MOL 1671  
DUPLICATE  
C3H7OH+R2OH=>H2O+R11C2H5+HCHO 4.0E+0005 2.000 -475.0 ! MOL 1672  
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y 6.0E+0011 0.000 17000.0 ! MOL 1673  
DUPLICATE  
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y 8.0E+0011 0.000 15500.0 ! MOL 1674  
DUPLICATE  
C3H7OH+R3OOH=>H2O2+R11C2H5+HCHO 5.4E+0004 2.000 15025.0 ! MOL 1675  
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y 3.0E-0001 4.000 8200.0 ! MOL 1676  
DUPLICATE  
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y 4.0E+0011 0.000 9600.0 ! MOL 1677  
DUPLICATE  
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO 3.9E+0004 2.000 7525.0 ! MOL 1678  
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y 1.6E+0011 0.000 7300.0 ! MOL 1679  
DUPLICATE  
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y 2.9E+0011 0.000 4500.0 ! MOL 1680  
DUPLICATE  
C3H7OH+R8CH3OO=>CH3OOH+R11C2H5+HCHO 0.0E+0000 0.000 0.0 ! MOL 1681

C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y	3.0E+0011	0.000	13500.0	! MOL 1682
DUPLICATE				
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y	4.0E+0011	0.000	11000.0	! MOL 1683
DUPLICATE				
C3H7OH+R11C2H5=>C2H6+R11C2H5+HCHO	2.3E+0004	2.000	10525.0	! MOL 1684
C3H8OL+R1H=>H2+R2OH+C3H6Y	2.9E+0007	2.000	7700.0	! MOL 1685
DUPLICATE				
C3H8OL+R1H=>H2+R2OH+C3H6Y	1.8E+0007	2.000	5000.0	! MOL 1686
DUPLICATE				
C3H8OL+R1H=>H2+R11C2H5+HCHO	2.4E+0006	2.000	6525.0	! MOL 1687
C3H8OL+R2OH=>H2O+R2OH+C3H6Y	2.7E+0006	2.000	450.0	! MOL 1688
DUPLICATE				
C3H8OL+R2OH=>H2O+R2OH+C3H6Y	5.2E+0006	2.000	-765.0	! MOL 1689
DUPLICATE				
C3H8OL+R2OH=>H2O+R11C2H5+HCHO	4.0E+0005	2.000	-475.0	! MOL 1690
C3H8OL+R3OOH=>H2O2+R2OH+C3H6Y	6.0E+0011	0.000	17000.0	! MOL 1691
DUPLICATE				
C3H8OL+R3OOH=>H2O2+R2OH+C3H6Y	8.0E+0011	0.000	15500.0	! MOL 1692
DUPLICATE				
C3H8OL+R3OOH=>H2O2+R11C2H5+HCHO	5.4E+0004	2.000	15025.0	! MOL 1693
C3H8OL+R4CH3=>CH4+R2OH+C3H6Y	3.0E-0001	4.000	8200.0	! MOL 1694
DUPLICATE				
C3H8OL+R4CH3=>CH4+R2OH+C3H6Y	4.0E+0011	0.000	9600.0	! MOL 1695
DUPLICATE				
C3H8OL+R4CH3=>CH4+R11C2H5+HCHO	3.9E+0004	2.000	7525.0	! MOL 1696
C3H8OL+R8CH3OO=>CH3OOH+R2OH+C3H6Y	1.6E+0011	0.000	7300.0	! MOL 1697
DUPLICATE				
C3H8OL+R8CH3OO=>CH3OOH+R2OH+C3H6Y	2.9E+0011	0.000	4500.0	! MOL 1698
DUPLICATE				
C3H8OL+R8CH3OO=>CH3OOH+R11C2H5+HCHO	0.0E+0000	0.000	0.0	! MOL 1699
C3H8OL+R11C2H5=>C2H6+R2OH+C3H6Y	3.0E+0011	0.000	13500.0	! MOL 1700
DUPLICATE				
C3H8OL+R11C2H5=>C2H6+R2OH+C3H6Y	4.0E+0011	0.000	11000.0	! MOL 1701
DUPLICATE				
C3H8OL+R11C2H5=>C2H6+R11C2H5+HCHO	2.3E+0004	2.000	10525.0	! MOL 1702
C4H10OL+R1H=>H2+R2OH+C4H8Z	2.9E+0007	2.000	7700.0	! MOL 1703
DUPLICATE				
C4H10OL+R1H=>H2+R2OH+C4H8Z	2.7E+0007	2.000	5000.0	! MOL 1704
DUPLICATE				
C4H10OL+R1H=>H2+R19C3H7+HCHO	2.4E+0006	2.000	6525.0	! MOL 1705
C4H10OL+R2OH=>H2O+R2OH+C4H8Z	2.7E+0006	2.000	450.0	! MOL 1706
DUPLICATE				
C4H10OL+R2OH=>H2O+R2OH+C4H8Z	7.8E+0006	2.000	-765.0	! MOL 1707
DUPLICATE				
C4H10OL+R2OH=>H2O+R19C3H7+HCHO	4.0E+0005	2.000	-475.0	! MOL 1708
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Z	6.0E+0011	0.000	17000.0	! MOL 1709
DUPLICATE				
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Z	1.2E+0012	0.000	15500.0	! MOL 1710
DUPLICATE				
C4H10OL+R3OOH=>H2O2+R19C3H7+HCHO	5.4E+0004	2.000	15025.0	! MOL 1711
C4H10OL+R4CH3=>CH4+R2OH+C4H8Z	3.0E-0001	4.000	8200.0	! MOL 1712
DUPLICATE				
C4H10OL+R4CH3=>CH4+R2OH+C4H8Z	6.0E+0011	0.000	9600.0	! MOL 1713
DUPLICATE				
C4H10OL+R4CH3=>CH4+R19C3H7+HCHO	3.9E+0004	2.000	7525.0	! MOL 1714

C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Z 1.6E+0011 0.000 7300.0 ! MOL  
 1715  
 DUPLICATE  
 C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Z 4.4E+0011 0.000 4500.0 ! MOL  
 1716  
 DUPLICATE  
 C4H10OL+R8CH3OO=>CH3OOH+R19C3H7+HCHO 0.0E+0000 0.000 0.0 ! MOL 1717  
 C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Z 3.0E+0011 0.000 13500.0 ! MOL 1718  
 DUPLICATE  
 C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Z 6.0E+0011 0.000 11000.0 ! MOL 1719  
 DUPLICATE  
 C4H10OL+R11C2H5=>C2H6+R19C3H7+HCHO 2.3E+0004 2.000 10525.0 ! MOL  
 1720  
 C3H7OH+B1O=>R2OH+R2OH+C3H6Y 3.9E+0013 0.000 5200.0 ! MOL 1721  
 DUPLICATE  
 C3H7OH+B1O=>R2OH+R2OH+C3H6Y 4.0E+0013 0.000 3280.0 ! MOL 1722  
 DUPLICATE  
 C3H7OH+B1O=>R2OH+R11C2H5+HCHO 1.3E+0006 2.000 5025.0 ! MOL 1723  
 C3H8OL+B1O=>R2OH+R2OH+C3H6Y 3.9E+0013 0.000 5200.0 ! MOL 1724  
 DUPLICATE  
 C3H8OL+B1O=>R2OH+R2OH+C3H6Y 4.0E+0013 0.000 3280.0 ! MOL 1725  
 DUPLICATE  
 C3H8OL+B1O=>R2OH+R11C2H5+HCHO 1.3E+0006 2.000 5025.0 ! MOL 1726  
 C4H10OL+B1O=>R2OH+R2OH+C4H8Y 3.9E+0013 0.000 5200.0 ! MOL 1727  
 DUPLICATE  
 C4H10OL+B1O=>R2OH+R2OH+C4H8Y 6.0E+0013 0.000 3280.0 ! MOL 1728  
 DUPLICATE  
 C4H10OL+B1O=>R2OH+R19C3H7+HCHO 1.3E+0006 2.000 5025.0 ! MOL 1729

! Aldehydes metathesis

C2H5CHO+R1H=>H2+RC3H5O 4.0E+0013 0.000 4200.0 ! \*2 1730  
 C2H5CHO+R2OH=>H2O+RC3H5O 4.2E+0012 0.000 500.0 ! \*2 1731  
 C2H5CHO+R3OOH=>H2O2+RC3H5O 1.0E+0012 0.000 10000.0 ! \*2 1732  
 C2H5CHO+R4CH3=>CH4+RC3H5O 2.0E-0006 5.600 2500.0 ! \*2 1733  
 C2H5CHO+R11C2H5=>C2H6+RC3H5O 1.3E+0012 0.000 8500.0 ! \*2 1734  
 C4H8OA+R1H=>H2+R80C4H7OK 4.0E+0013 0.000 4200.0 ! \*2 1735  
 C4H8OA+R2OH=>H2O+R80C4H7OK 4.2E+0012 0.000 500.0 ! \*2 1736  
 C4H8OA+R3OOH=>H2O2+R80C4H7OK 1.0E+0012 0.000 10000.0 ! \*2 1737  
 C4H8OA+R4CH3=>CH4+R80C4H7OK 2.0E-0006 5.600 2500.0 ! \*2 1738  
 C4H8OA+R11C2H5=>C2H6+R80C4H7OK 1.3E+0012 0.000 8500.0 ! \*2 1739  
 C5H10OA+R1H=>H2+RC5H9O 4.0E+0013 0.000 4200.0 ! \*2 1740  
 C5H10OA+R2OH=>H2O+RC5H9O 4.2E+0012 0.000 500.0 ! \*2 1741  
 C5H10OA+R3OOH=>H2O2+RC5H9O 1.0E+0012 0.000 10000.0 ! \*2 1742  
 C5H10OA+R4CH3=>CH4+RC5H9O 2.0E-0006 5.600 2500.0 ! \*2 1743  
 C5H10OA+R11C2H5=>C2H6+RC5H9O 1.3E+0012 0.000 8500.0 ! \*2 1744  
 !C6H10OAZ+R1H=>H2+RC6H9OZ 4.0E+0013 0.000 4200.0 ! \*2 1745  
 !C6H10OAZ+R2OH=>H2O+RC6H9OZ 4.2E+0012 0.000 500.0 ! \*2 1746  
 !C6H10OAZ+R3OOH=>H2O2+RC6H9OZ 1.0E+0012 0.000 10000.0 ! \*2 1747  
 !C6H10OAZ+R4CH3=>CH4+RC6H9OZ 2.0E-0006 5.600 2500.0 ! \*2 1748  
 !C6H10OAZ+R11C2H5=>C2H6+RC6H9OZ 1.3E+0012 0.000 8500.0 ! \*2 1749  
 C5H8OAZ+R1H=>H2+RC5H7OZ 4.0E+0013 0.000 4200.0 ! \*2 1750  
 C5H8OAZ+R2OH=>H2O+RC5H7OZ 4.2E+0012 0.000 500.0 ! \*2 1751  
 C5H8OAZ+R3OOH=>H2O2+RC5H7OZ 1.0E+0012 0.000 10000.0 ! \*2 1752  
 C5H8OAZ+R4CH3=>CH4+RC5H7OZ 2.0E-0006 5.600 2500.0 ! \*2 1753  
 C5H8OAZ+R11C2H5=>C2H6+RC5H7OZ 1.3E+0012 0.000 8500.0 ! \*2 1754  
 C4H6OAZ+R1H=>H2+RC4H5OZ 4.0E+0013 0.000 4200.0 ! \*2 1755  
 C4H6OAZ+R2OH=>H2O+RC4H5OZ 4.2E+0012 0.000 500.0 ! \*2 1756  
 C4H6OAZ+R3OOH=>H2O2+RC4H5OZ 1.0E+0012 0.000 10000.0 ! \*2 1757

C4H6OAZ+R4CH3=>CH4+RC4H5OZ 2.0E-0006 5.600 2500.0 ! \*2 1758  
C4H6OAZ+R11C2H5=>C2H6+RC4H5OZ 1.3E+0012 0.000 8500.0 ! \*2 1759  
C6H12OAZ+R1H=>H2+R29C6H11OK 4.0E+0013 0.000 4200.0 ! \*2 1760  
C6H12OAZ+R2OH=>H2O+R29C6H11OK 4.2E+0012 0.000 500.0 ! \*2 1761  
C6H12OAZ+R3OOH=>H2O2+R29C6H11OK 1.0E+0012 0.000 10000.0 ! \*2 1762  
C6H12OAZ+R4CH3=>CH4+R29C6H11OK 2.0E-0006 5.600 2500.0 ! \*2 1763  
C6H12OAZ+R11C2H5=>C2H6+R29C6H11OK 1.3E+0012 0.000 8500.0 ! \*2 1764  
C7H14OAZ+R1H=>H2+RC7H13O 4.0E+0013 0.000 4200.0 ! \*2 1765  
C7H14OAZ+R2OH=>H2O+RC7H13O 4.2E+0012 0.000 500.0 ! \*2 1766  
C7H14OAZ+R3OOH=>H2O2+RC7H13O 1.0E+0012 0.000 10000.0 ! \*2 1767  
C7H14OAZ+R4CH3=>CH4+RC7H13O 2.0E-0006 5.600 2500.0 ! \*2 1768  
C7H14OAZ+R11C2H5=>C2H6+RC7H13O 1.3E+0012 0.000 8500.0 ! \*2 1769

C4H6OAY+R1H=>H2+R10C2H3V+CH2COZ 4.0E+0013 0.000 4200.0 ! \*1 1770  
C4H6OAY+R2OH=>H2O+R10C2H3V+CH2COZ 4.0E+0012 0.000 500.0 ! \*1 1771  
C4H6OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ 1.0E+0012 0.000 10000.0 ! \*1  
1772  
C4H6OAY+R4CH3=>CH4+R10C2H3V+CH2COZ 2.0E-0006 0.000 2500.0 ! \*1 1773  
C4H6OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ 1.3E+0012 0.000 8500.0 ! \*1  
1774  
C5H8OAY+R1H=>H2+RC3H5Y+CH2COZ 4.0E+0013 0.000 4200.0 ! \*1 1775  
C5H8OAY+R2OH=>H2O+RC3H5Y+CH2COZ 4.0E+0012 0.000 500.0 ! \*1 1776  
C5H8OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ 1.0E+0012 0.000 10000.0 ! \*1 1777  
C5H8OAY+R4CH3=>CH4+RC3H5Y+CH2COZ 2.0E-0006 0.000 2500.0 ! \*1 1778  
C5H8OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ 1.3E+0012 0.000 8500.0 ! \*1  
1779  
C6H10OAY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z 4.0E+0013 0.000 4200.0 ! \*1  
1780  
C6H10OAY+R2OH=>H2O+R10C2H3V+CH2COZ+C2H4Z 4.0E+0012 0.000 500.0 ! \*1  
1781  
C6H10OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+C2H4Z 1.0E+0012 0.000 10000.0  
! \*1 1782  
C6H10OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z 2.0E-0006 0.000 2500.0 !  
\*1 1783  
C6H10OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z 1.3E+0012 0.000 8500.0  
! \*1 1784

! Keto radicals decomposition

RC3H5O=>B2CO+R11C2H5 1.8E+0014 0.000 15600.0 ! COR 1785  
RC5H9O=>B2CO+R20C4H9 1.8E+0014 0.000 15600.0 ! COR 1786  
RC7H13O=>B2CO+R11C2H5+2C2H4Z 1.8E+0014 0.000 15600.0 ! COR 1787  
RC6H9OZ=>C2H2T+B2CO+R4CH3+C2H4Z 1.8E+0014 0.000 15600.0 ! COR 1788  
RC5H7OZ=>B2CO+R10C2H3V+C2H4Z 1.8E+0014 0.000 15600.0 ! COR 1789  
RC4H5OZ=>C2H2T+B2CO+R4CH3 1.8E+0014 0.000 15600.0 ! COR 1790

! keto radicals addition to O2

RC3H5O+O2=>RC3H5O3 3.0E+0019 -2.500 0.0 ! COR 1791  
RC5H9O+O2=>RC5H9O3 3.0E+0019 -2.500 0.0 ! COR 1792  
RC6H9OZ+O2=>RC6H9O3Z 3.0E+0019 -2.500 0.0 ! COR 1793  
RC5H7OZ+O2=>RC5H7O3Z 3.0E+0019 -2.500 0.0 ! COR 1794  
RC4H5OZ+O2=>RC4H5O3Z 3.0E+0019 -2.500 0.0 ! COR 1795  
RC7H13O+O2=>RC7H13O3 3.0E+0019 -2.500 0.0 ! COR 1796

! Peracide radical decomposition

RC3H5O3=>C2H4Z+R2OH +CO2 4.5E+0011 0.000 25000.0 ! PER 1797  
RC5H9O3=>C4H8Y+R2OH+CO2 4.5E+0011 0.000 25000.0 ! PER 1798  
RC6H9O3Z=>C5H8Z2+R2OH+CO2 4.5E+0011 0.000 25000.0 ! PER 1799



RC5H7O3Z=>C4H6Z2+R2OH+CO2	4.5E+0011	0.000	25000.0	! PER 1800
RC4H5O3Z=>C3H4Z2+R2OH+CO2	4.5E+0011	0.000	25000.0	! PER 1801
RC7H13O3=>C6H12Z+R2OH+CO2	4.5E+0011	0.000	25000.0	! PER 1802

! Ketones reactions

C2H6CO+R1H=>H2+CH2COZ+R4CH3	5.7E+0007	2.000	7700.0	! MK 1803
C2H6CO+R2OH=>H2O+CH2COZ+R4CH3	5.4E+0006	2.000	450.0	! MK 1804
C2H6CO+R3OOH=>H2O2+CH2COZ+R4CH3	1.2E+0012	0.000	17000.0	! MK 1805
C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3	6.0E-0001	4.000	8200.0	! MK 1806
C2H6CO+R8CH3OO=>CH3OOH+CH2COZ+R4CH3	1.2E+0013	0.000	20000.0	! MK 1807
C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3	6.0E+0011	0.000	13500.0	! MK 1808
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	5.7E+0007	2.000	7700.0	! MK 1809
DUPLICATE				
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	9.0E+0006	2.000	5000.0	! MK 1810
DUPLICATE				
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5	5.4E+0006	2.000	450.0	! MK 1811
DUPLICATE				
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5	2.6E+0006	2.000	-765.0	! MK 1812
DUPLICATE				
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5	1.2E+0012	0.000	17000.0	! MK 1813
DUPLICATE				
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5	4.0E+0011	0.000	15500.0	! MK 1814
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	6.0E-0001	4.000	8200.0	! MK 1815
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	2.0E+0011	0.000	9600.0	! MK 1816
DUPLICATE				
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5	1.2E+0013	0.000	20000.0	! MK 1817
DUPLICATE				
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5	3.0E+0012	0.000	17500.0	! MK 1818
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	6.0E+0011	0.000	13500.0	! MK 1819
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	2.0E+0011	0.000	11000.0	! MK 1820
DUPLICATE				
C5H10OK+R1H=>H2+CH2COZ+R19C3H7	5.7E+0007	2.000	7700.0	! MK 1821
DUPLICATE				
C5H10OK+R1H=>H2+CH2COZ+R19C3H7	1.8E+0007	2.000	5000.0	! MK 1822
DUPLICATE				
C5H10OK+R2OH=>H2O+CH2COZ+R19C3H7	5.4E+0006	2.000	450.0	! MK 1823
DUPLICATE				
C5H10OK+R2OH=>H2O+CH2COZ+R19C3H7	5.2E+0006	2.000	-765.0	! MK 1824
DUPLICATE				
C5H10OK+R3OOH=>H2O2+CH2COZ+R19C3H7	1.2E+0012	0.000	17000.0	! MK 1825
DUPLICATE				
C5H10OK+R3OOH=>H2O2+CH2COZ+R19C3H7	8.0E+0011	0.000	15500.0	! MK 1826
DUPLICATE				
C5H10OK+R4CH3=>CH4+CH2COZ+R19C3H7	6.0E-0001	4.000	8200.0	! MK 1827
DUPLICATE				
C5H10OK+R4CH3=>CH4+CH2COZ+R19C3H7	4.0E+0011	0.000	9600.0	! MK 1828
DUPLICATE				

C5H10OK+R8CH3OO=>CH3OOH+CH2COZ+R19C3H7 1.2E+0013 0.000 20000.0 ! MK  
 1829  
 DUPLICATE  
 C5H10OK+R8CH3OO=>CH3OOH+CH2COZ+R19C3H7 6.0E+0012 0.000 17500.0 ! MK  
 1830  
 DUPLICATE  
 C5H10OK+R11C2H5=>C2H6+CH2COZ+R19C3H7 6.0E+0011 0.000 13500.0 ! MK  
 1831  
 DUPLICATE  
 C5H10OK+R11C2H5=>C2H6+CH2COZ+R19C3H7 4.0E+0011 0.000 11000.0 ! MK  
 1832  
 DUPLICATE  
 M39C6H10OKZ+R1H=>H2+RC4H7Y+CH2COZ 2.9E+0007 2.000 7700.0 ! MKZ 1833  
 M39C6H10OKZ+R2OH=>H2O+RC4H7Y+CH2COZ 2.7E+0006 2.000 450.0 ! MKZ  
 1834  
 M39C6H10OKZ+R3OOH=>H2O2+RC4H7Y+CH2COZ 6.0E+0011 0.000 17000.0 ! MKZ  
 1835  
 M39C6H10OKZ+R4CH3=>CH4+RC4H7Y+CH2COZ 3.0E-0001 4.000 8200.0 ! MKZ  
 1836  
 M39C6H10OKZ+R8CH3OO=>CH3OOH+RC4H7Y+CH2COZ 6.0E+0012 0.000 20000.0 !  
 MKZ 1837  
 M39C6H10OKZ+R11C2H5=>C2H6+RC4H7Y+CH2COZ 3.0E+0011 0.000 13500.0 !  
 MKZ 1838  
 C3H4OKZ+R1H=>H2+R10C2H3V+B2CO 2.9E+0007 2.000 7700.0 ! MKZ 1839  
 C3H4OKZ+R2OH=>H2O+R10C2H3V+B2CO 2.7E+0006 2.000 450.0 ! MKZ 1840  
 C3H4OKZ+R3OOH=>H2O2+R10C2H3V+B2CO 6.0E+0011 0.000 17000.0 ! MKZ  
 1841  
 C3H4OKZ+R4CH3=>CH4+R10C2H3V+B2CO 3.0E-0001 4.000 8200.0 ! MKZ 1842  
 C3H4OKZ+R8CH3OO=>CH3OOH+R10C2H3V+B2CO 6.0E+0012 0.000 20000.0 ! MKZ  
 1843  
 C3H4OKZ+R11C2H5=>C2H6+R10C2H3V+B2CO 3.0E+0011 0.000 13500.0 ! MKZ  
 1844  
 C4H6OKZ+R1H=>H2+R10C2H3V+CH2COZ 2.9E+0007 2.000 7700.0 ! MKZ 1845  
 C4H6OKZ+R2OH=>H2O+R10C2H3V+CH2COZ 2.7E+0006 2.000 450.0 ! MKZ 1846  
 C4H6OKZ+R3OOH=>H2O2+R10C2H3V+CH2COZ 6.0E+0011 0.000 17000.0 ! MKZ  
 1847  
 C4H6OKZ+R4CH3=>CH4+R10C2H3V+CH2COZ 3.0E-0001 4.000 8200.0 ! MKZ  
 1848  
 C4H6OKZ+R8CH3OO=>CH3OOH+R10C2H3V+CH2COZ 6.0E+0012 0.000 20000.0 !  
 MKZ 1849  
 C4H6OKZ+R11C2H5=>C2H6+R10C2H3V+CH2COZ 3.0E+0011 0.000 13500.0 ! MKZ  
 1850

! Unsaturated ester reactions  
 ! Esters metatesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis  
 ! Addition on unsaturated esters

! Carboxylic acid reactions  
 ! Carboxylic acid metathesis

M40C6H10O2ZB+R1H=>H2+CO2+R4CH3+C4H6Z2 4.2E+0006 2.100 6900.0 ! MZB  
 1851

M40C6H10O2ZB+R1H=>H2+C4H6Z2+R23C2H3O2B MZB 1852	5.4E+0004	2.500	-1900.0	!
M40C6H10O2ZB+R1H=>H2+C4H6O2ZB+R10C2H3V 1853	1.8E+0007	2.000	5000.0	! MZB
M40C6H10O2ZB+R2OH=>H2O+CO2+R4CH3+C4H6Z2 MZB 1854	5.4E+0004	2.000	-340.0	!
M40C6H10O2ZB+R2OH=>H2O+C4H6Z2+R23C2H3O2B MZB 1855	3.0E+0006	2.000	-1520.0	!
M40C6H10O2ZB+R2OH=>H2O+C4H6O2ZB+R10C2H3V MZB 1856	5.2E+0006	2.000	-765.0	!
M40C6H10O2ZB+R3OOH=>H2O2+CO2+R4CH3+C4H6Z2 MZB 1857	1.0E+0011	0.000	11500.0	!
M40C6H10O2ZB+R3OOH=>H2O2+C4H6Z2+R23C2H3O2B ! MZB 1858	6.4E+0003	2.600	12400.0	
M40C6H10O2ZB+R3OOH=>H2O2+C4H6O2ZB+R10C2H3V ! MZB 1859	8.0E+0011	0.000	15500.0	
M40C6H10O2ZB+R4CH3=>CH4+CO2+R4CH3+C4H6Z2 MZB 1860	1.4E+0001	3.100	9940.0	!
M40C6H10O2ZB+R4CH3=>CH4+C4H6Z2+R23C2H3O2B MZB 1861	1.0E+0011	0.000	7300.0	!
M40C6H10O2ZB+R4CH3=>CH4+C4H6O2ZB+R10C2H3V MZB 1862	4.0E+0011	0.000	9600.0	!
M40C6H10O2ZB+R8CH3OO=>CH3OOH+CO2+R4CH3+C4H6Z2 13500.0 ! MZB 1863	1.0E+0012	0.000		
M40C6H10O2ZB+R8CH3OO=>CH3OOH+C4H6Z2+R23C2H3O2B 14550.0 ! MZB 1864	1.0E+0012	0.000		
M40C6H10O2ZB+R8CH3OO=>CH3OOH+C4H6O2ZB+R10C2H3V 17500.0 ! MZB 1865	6.0E+0012	0.000		
M40C6H10O2ZB+R11C2H5=>C2H6+CO2+R4CH3+C4H6Z2 ! MZB 1866	1.4E+0001	3.100	8940.0	
M40C6H10O2ZB+R11C2H5=>C2H6+C4H6Z2+R23C2H3O2B ! MZB 1867	1.5E+0000	3.500	4140.0	
M40C6H10O2ZB+R11C2H5=>C2H6+C4H6O2ZB+R10C2H3V ! MZB 1868	4.0E+0011	0.000	11000.0	
C5H8O2ZB+R1H=>H2+CO2+R1H+C4H6Z2	4.2E+0006	2.100	6900.0	! MZB 1869
C5H8O2ZB+R1H=>H2+C4H6Z2+R22CO2H	5.4E+0004	2.500	-1900.0	! MZB 1870
C5H8O2ZB+R1H=>H2+C3H4O2ZB+R10C2H3V 1871	9.0E+0006	2.000	5000.0	! MZB
C5H8O2ZB+R2OH=>H2O+CO2+R1H+C4H6Z2	5.4E+0004	2.000	-340.0	! MZB 1872
C5H8O2ZB+R2OH=>H2O+C4H6Z2+R22CO2H 1873	3.0E+0006	2.000	-1520.0	! MZB
C5H8O2ZB+R2OH=>H2O+C3H4O2ZB+R10C2H3V 1874	2.6E+0006	2.000	-765.0	! MZB
C5H8O2ZB+R3OOH=>H2O2+CO2+R1H+C4H6Z2 1875	1.0E+0011	0.000	11500.0	! MZB
C5H8O2ZB+R3OOH=>H2O2+C4H6Z2+R22CO2H 1876	6.4E+0003	2.600	12400.0	! MZB
C5H8O2ZB+R3OOH=>H2O2+C3H4O2ZB+R10C2H3V MZB 1877	4.0E+0011	0.000	15500.0	!
C5H8O2ZB+R4CH3=>CH4+CO2+R1H+C4H6Z2 1878	1.4E+0001	3.100	9940.0	! MZB
C5H8O2ZB+R4CH3=>CH4+C4H6Z2+R22CO2H 1879	1.0E+0011	0.000	7300.0	! MZB
C5H8O2ZB+R4CH3=>CH4+C3H4O2ZB+R10C2H3V 1880	2.0E+0011	0.000	9600.0	! MZB
C5H8O2ZB+R8CH3OO=>CH3OOH+CO2+R1H+C4H6Z2 MZB 1881	1.0E+0012	0.000	13500.0	!

C5H8O2ZB+R8CH3OO=>CH3OOH+C4H6Z2+R22CO2H	1.0E+0012	0.000	14550.0	!
MZB 1882				
C5H8O2ZB+R8CH3OO=>CH3OOH+C3H4O2ZB+R10C2H3V	3.0E+0012	0.000	17500.0	!
MZB 1883				
C5H8O2ZB+R11C2H5=>C2H6+CO2+R1H+C4H6Z2	1.4E+0001	3.100	8940.0	!
MZB 1884				
C5H8O2ZB+R11C2H5=>C2H6+C4H6Z2+R22CO2H	1.5E+0000	3.500	4140.0	!
MZB 1885				
C5H8O2ZB+R11C2H5=>C2H6+C3H4O2ZB+R10C2H3V	2.0E+0011	0.000	11000.0	!
MZB 1886				
C4H6O2ZB+R1H=>H2+CO2+RC3H5Y	4.2E+0006	2.100	6900.0	!
MZB 1887				
DUPLICATE				
C4H6O2ZB+R1H=>H2+CO2+RC3H5Y	5.4E+0004	2.500	-1900.0	!
MZB 1888				
DUPLICATE				
C4H6O2ZB+R2OH=>H2O+CO2+RC3H5Y	5.4E+0004	2.000	-340.0	!
MZB 1889				
DUPLICATE				
C4H6O2ZB+R2OH=>H2O+CO2+RC3H5Y	3.0E+0006	2.000	-1520.0	!
MZB 1890				
DUPLICATE				
C4H6O2ZB+R3OOH=>H2O2+CO2+RC3H5Y	1.0E+0011	0.000	11500.0	!
MZB 1891				
DUPLICATE				
C4H6O2ZB+R3OOH=>H2O2+CO2+RC3H5Y	6.4E+0003	2.600	12400.0	!
MZB 1892				
DUPLICATE				
C4H6O2ZB+R4CH3=>CH4+CO2+RC3H5Y	1.4E+0001	3.100	9940.0	!
MZB 1893				
DUPLICATE				
C4H6O2ZB+R4CH3=>CH4+CO2+RC3H5Y	1.0E+0011	0.000	7300.0	!
MZB 1894				
DUPLICATE				
C4H6O2ZB+R8CH3OO=>CH3OOH+CO2+RC3H5Y	1.0E+0012	0.000	13500.0	!
MZB 1895				
DUPLICATE				
C4H6O2ZB+R8CH3OO=>CH3OOH+CO2+RC3H5Y	1.0E+0012	0.000	14550.0	!
MZB 1896				
DUPLICATE				
C4H6O2ZB+R11C2H5=>C2H6+CO2+RC3H5Y	1.4E+0001	3.100	8940.0	!
MZB 1897				
DUPLICATE				
C4H6O2ZB+R11C2H5=>C2H6+CO2+RC3H5Y	7.4E-0001	3.500	4140.0	!
MZB 1898				
DUPLICATE				
C3H4O2ZB+R1H=>H2+CO2+R10C2H3V	4.2E+0006	2.100	6900.0	!
MZB 1899				
C3H4O2ZB+R2OH=>H2O+CO2+R10C2H3V	5.4E+0004	2.000	-340.0	!
MZB 1900				
C3H4O2ZB+R3OOH=>H2O2+CO2+R10C2H3V	1.0E+0011	0.000	11500.0	!
MZB 1901				
C3H4O2ZB+R4CH3=>CH4+CO2+R10C2H3V	1.4E+0001	3.100	9940.0	!
MZB 1902				
C3H4O2ZB+R8CH3OO=>CH3OOH+CO2+R10C2H3V	1.0E+0012	0.000	13500.0	!
MZB 1903				
C3H4O2ZB+R11C2H5=>C2H6+CO2+R10C2H3V	1.4E+0001	3.100	8940.0	!
MZB 1904				
C6H10O3AB+R1H=>H2+B2CO+R246C5H9O2B	4.0E+0013	0.000	4200.0	!
MAB 1905				
C6H10O3AB+R2OH=>H2O+B2CO+R246C5H9O2B	4.2E+0012	0.000	500.0	!
MAB 1906				
C6H10O3AB+R3OOH=>H2O2+B2CO+R246C5H9O2B	1.0E+0012	0.000	10000.0	!
MAB 1907				
C6H10O3AB+R4CH3=>CH4+B2CO+R246C5H9O2B	2.0E-0006	5.600	2500.0	!
MAB 1908				
C6H10O3AB+R8CH3OO=>CH3OOH+B2CO+R246C5H9O2B	2.0E-0006	5.600	2500.0	!
MAB 1909				
C6H10O3AB+R11C2H5=>C2H6+B2CO+R246C5H9O2B	1.3E+0012	0.000	8500.0	!
MAB 1910				
C4H6O3AB+R1H=>H2+B2CO+R56C3H5O2B	4.0E+0013	0.000	4200.0	!
MAB 1911				

C4H6O3AB+R2OH=>H2O+B2CO+R56C3H5O2B 4.2E+0012 0.000 500.0 ! MAB 1912  
 C4H6O3AB+R3OOH=>H2O2+B2CO+R56C3H5O2B 1.0E+0012 0.000 10000.0 ! MAB  
 1913  
 C4H6O3AB+R4CH3=>CH4+B2CO+R56C3H5O2B 2.0E-0006 5.600 2500.0 ! MAB  
 1914  
 C4H6O3AB+R8CH3OO=>CH3OOH+B2CO+R56C3H5O2B 2.0E-0006 5.600 2500.0 !  
 MAB 1915  
 C4H6O3AB+R11C2H5=>C2H6+B2CO+R56C3H5O2B 1.3E+0012 0.000 8500.0 ! MAB  
 1916  
 C3H4O3AB+R1H=>H2+B2CO+R23C2H3O2B 4.0E+0013 0.000 4200.0 ! MAB 1917  
 C3H4O3AB+R2OH=>H2O+B2CO+R23C2H3O2B 4.2E+0012 0.000 500.0 ! MAB 1918  
 C3H4O3AB+R3OOH=>H2O2+B2CO+R23C2H3O2B 1.0E+0012 0.000 10000.0 ! MAB  
 1919  
 C3H4O3AB+R4CH3=>CH4+B2CO+R23C2H3O2B 2.0E-0006 5.600 2500.0 ! MAB  
 1920  
 C3H4O3AB+R8CH3OO=>CH3OOH+B2CO+R23C2H3O2B 2.0E-0006 5.600 2500.0 !  
 MAB 1921  
 C3H4O3AB+R11C2H5=>C2H6+B2CO+R23C2H3O2B 1.3E+0012 0.000 8500.0 ! MAB  
 1922

! Carboxylic acid decomposition

C6H12O4PB=>R2OH+R56C3H5O2B+C2H5CHO 1.5E+0016 0.000 43000.0 ! DPB  
 1923  
 C4H8O4PB=>R2OH+R23C2H3O2B+CH3CHO 1.5E+0016 0.000 43000.0 ! DPB 1924  
 C3H6O4PB=>R2OH+R23C2H3O2B+HCHO 1.5E+0016 0.000 43000.0 ! DPB 1925  
 C6H10O5KPB=>R2OH+B2CO+R56C3H5O2B+CH3CHO 1.5E+0016 0.000 43000.0 !  
 KPB 1926  
 C4H6O5KPB=>R2OH+B2CO+R23C2H3O2B+HCHO 1.5E+0016 0.000 43000.0 ! KPB  
 1927  
 C3H4O5KPB=>R2OH+B2CO+R22CO2H+HCHO 1.5E+0016 0.000 43000.0 ! KPB  
 1928

! Alkohol ene to dienes

C3H6OLY+R1H=>H2+HCHO+R10C2H3V 5.4E+0004 2.500 -1900.0 ! ROH 1929  
 C3H6OLY+R2OH=>H2O+HCHO+R10C2H3V 3.0E+0006 2.000 -1520.0 ! ROH 1930  
 C3H6OLY+R3OOH=>H2O2+HCHO+R10C2H3V 6.4E+0003 2.600 12400.0 ! ROH  
 1931  
 C3H6OLY+R4CH3=>CH4+HCHO+R10C2H3V 1.0E+0011 0.000 7300.0 ! ROH 1932  
 C3H6OLY+R8CH3OO=>CH3OOH+HCHO+R10C2H3V 1.0E+0012 0.000 14550.0 ! ROH  
 1933  
 C3H6OLY+R11C2H5=>C2H6+HCHO+R10C2H3V 1.5E+0000 3.500 4140.0 ! ROH  
 1934  
 C4H8OLY+R1H=>H2+HCHO+RC3H5Y 5.4E+0004 2.500 -1900.0 ! ROH 1935  
 C4H8OLY+R2OH=>H2O+HCHO+RC3H5Y 3.0E+0006 2.000 -1520.0 ! ROH 1936  
 C4H8OLY+R3OOH=>H2O2+HCHO+RC3H5Y 6.4E+0003 2.600 12400.0 ! ROH 1937  
 C4H8OLY+R4CH3=>CH4+HCHO+RC3H5Y 1.0E+0011 0.000 7300.0 ! ROH 1938  
 C4H8OLY+R8CH3OO=>CH3OOH+HCHO+RC3H5Y 1.0E+0012 0.000 14550.0 ! ROH  
 1939  
 C4H8OLY+R11C2H5=>C2H6+HCHO+RC3H5Y 1.5E+0000 3.500 4140.0 ! ROH 1940  
 C5H10OLY+R1H=>H2+HCHO+RC4H7Y 5.4E+0004 2.500 -1900.0 ! ROH 1941  
 C5H10OLY+R2OH=>H2O+HCHO+RC4H7Y 3.0E+0006 2.000 -1520.0 ! ROH 1942  
 C5H10OLY+R3OOH=>H2O2+HCHO+RC4H7Y 6.4E+0003 2.600 12400.0 ! ROH 1943  
 C5H10OLY+R4CH3=>CH4+HCHO+RC4H7Y 1.0E+0011 0.000 7300.0 ! ROH 1944  
 C5H10OLY+R8CH3OO=>CH3OOH+HCHO+RC4H7Y 1.0E+0012 0.000 14550.0 ! ROH  
 1945  
 C5H10OLY+R11C2H5=>C2H6+HCHO+RC4H7Y 1.5E+0000 3.500 4140.0 ! ROH  
 1946  
 C6H12OLY+R1H=>H2+HCHO+RC5H9Y 5.4E+0004 2.500 -1900.0 ! ROH 1947

C6H12OLY+R2OH=>H2O+HCHO+RC5H9Y 3.0E+0006 2.000 -1520.0 ! ROH 1948  
C6H12OLY+R3OOH=>H2O2+HCHO+RC5H9Y 6.4E+0003 2.600 12400.0 ! ROH 1949  
C6H12OLY+R4CH3=>CH4+HCHO+RC5H9Y 1.0E+0011 0.000 7300.0 ! ROH 1950  
C6H12OLY+R8CH3OO=>CH3OOH+HCHO+RC5H9Y 1.0E+0012 0.000 14550.0 ! ROH  
1951  
C6H12OLY+R11C2H5=>C2H6+HCHO+RC5H9Y 1.5E+0000 3.500 4140.0 ! ROH  
1952

! Additions on dienes

C4H6Z2-13+R2OH=>RC3H5Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1953  
C4H6Z2+R2OH=>RC3H5Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1954  
C5H8Z2+R2OH=>RC4H7Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1955  
C3H4Z2+R2OH=>R10C2H3V+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1956  
C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V 1.0E+0005 2.500 -1900.0 ! AD 1957  
C6H10Y2+R2OH=>H2O+C4H6Z2+R10C2H3V 6.0E+0006 2.000 -1520.0 ! AD 1958  
C6H10Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V 1.2E+0004 2.600 12400.0 ! AD  
1959  
C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD 1960  
C6H10Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD  
1961  
C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V 3.0E+0000 3.500 4140.0 ! AD  
1962  
C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y 1.0E+0005 2.500 -1900.0 ! AD 1963  
C7H12Y2+R2OH=>H2O+C4H6Z2+RC3H5Y 6.0E+0006 2.000 -1520.0 ! AD 1964  
C7H12Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y 1.2E+0004 2.600 12400.0 ! AD 1965  
C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD 1966  
C7H12Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD  
1967  
C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y 3.0E+0000 3.500 4140.0 ! AD  
1968  
C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
1969  
C8H14Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+C2H4Z 6.0E+0006 2.000 -1520.0 !  
AD 1970  
C8H14Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+C2H4Z 1.2E+0004 2.600 12400.0 !  
AD 1971  
C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000 7300.0 !  
AD 1972  
C8H14Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000 7300.0  
! AD 1973  
C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z 3.0E+0000 3.500 4140.0  
! AD 1974  
C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
1975  
C9H16Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+C2H4Z 6.0E+0006 2.000 -1520.0 ! AD  
1976  
C9H16Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+C2H4Z 1.2E+0004 2.600 12400.0 !  
AD 1977  
C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0 ! AD  
1978  
C9H16Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0  
! AD 1979  
C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z 3.0E+0000 3.500 4140.0 !  
AD 1980  
C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z 1.0E+0005 2.500 -1900.0 !  
AD 1981  
C10H18Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+C2H4Z 6.0E+0006 2.000 -1520.0 !  
AD 1982

C10H18Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z 1.2E+0004 2.600 12400.0  
! AD 1983  
C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000 7300.0 !  
AD 1984  
C10H18Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
7300.0 ! AD 1985  
C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z 3.0E+0000 3.500 4140.0  
! AD 1986

! Diels Alder

! .Y termination

RC3H5Y+R1H=>C3H6Y 1.0E+0013 0.000 0.0 ! TER 1987  
RC3H5Y+R2OH=>C3H6OLY 1.0E+0013 0.000 0.0 ! TER 1988  
RC3H5Y+R3OOH=>C3H6O2PY 5.0E+0012 0.000 0.0 ! TER 1989  
RC3H5Y+R4CH3=>C4H8Y 1.0E+0013 0.000 0.0 ! TER 1990  
RC3H5Y+R5CHO=>C4H6OAY 1.0E+0013 0.000 0.0 ! TER 1991  
RC3H5Y+R6CH2OH=>C4H8OLY 1.0E+0013 0.000 0.0 ! TER 1992  
RC3H5Y+R8CH3OO=>HCHO+R7CH3O+R10C2H3V 1.0E+0013 0.000 0.0 ! TER 1993  
RC3H5Y+R11C2H5=>M31C5H10Y 1.0E+0013 0.000 0.0 ! TER 1994  
RC4H7Y+R1H=>C4H8Y 1.0E+0013 0.000 0.0 ! TER 1995  
RC4H7Y+R2OH=>C4H8OLY 1.0E+0013 0.000 0.0 ! TER 1996  
RC4H7Y+R3OOH=>C4H8O2PY 5.0E+0012 0.000 0.0 ! TER 1997  
RC4H7Y+R4CH3=>M31C5H10Y 1.0E+0013 0.000 0.0 ! TER 1998  
RC4H7Y+R5CHO=>C5H8OAY 1.0E+0013 0.000 0.0 ! TER 1999  
RC4H7Y+R6CH2OH=>C5H10OLY 1.0E+0013 0.000 0.0 ! TER 2000  
RC4H7Y+R8CH3OO=>HCHO+R7CH3O+RC3H5Y 1.0E+0013 0.000 0.0 ! TER 2001  
RC4H7Y+R11C2H5=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 2002  
RC5H9Y+R1H=>M31C5H10Y 1.0E+0013 0.000 0.0 ! TER 2003  
RC5H9Y+R2OH=>C5H10OLY 1.0E+0013 0.000 0.0 ! TER 2004  
RC5H9Y+R3OOH=>C5H10O2PY 5.0E+0012 0.000 0.0 ! TER 2005  
RC5H9Y+R4CH3=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 2006  
RC5H9Y+R5CHO=>C6H10OAY 1.0E+0013 0.000 0.0 ! TER 2007  
RC5H9Y+R6CH2OH=>C6H12OLY 1.0E+0013 0.000 0.0 ! TER 2008  
RC5H9Y+R8CH3OO=>HCHO+R7CH3O+RC4H7Y 1.0E+0013 0.000 0.0 ! TER 2009  
RC5H9Y+R11C2H5=>C7H14Z 1.0E+0013 0.000 0.0 ! TER 2010  
RC3H5Y+RC3H5Y=>C6H10Y2 1.0E+0013 0.000 0.0 ! TER 2011  
RC3H5Y+RC4H7Y=>C7H12Y2 1.0E+0013 0.000 0.0 ! TER 2012  
RC3H5Y+RC5H9Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 2013  
RC4H7Y+RC4H7Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 2014  
RC4H7Y+RC5H9Y=>C9H16Y2 1.0E+0013 0.000 0.0 ! TER 2015  
RC5H9Y+RC5H9Y=>C10H18Y2 1.0E+0013 0.000 0.0 ! TER 2016

! Pascal C0 C2 lumped data base

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! VERSION X.X 01/2002

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

! REACTIONS DE H2!

R1H+R1H+M=H2+M 1.87E18 -1.00 0.0 !(1,-  
1)<BAULCH94>!

O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ H2/0.0/  
C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/

! REACTIONS DE B4CH!

B4CH+R1H=B3C+H2                    7.8E13            0.            0.            !(2,-  
 2)<PEETERS97>!  
  
 !REACTIONS DE B6CH2!  
 B6CH2+M=B5CH2+M                    1.51E13            0.0            0.0            !(3,-  
 3)<BAULCH94>!  
     N2/.4/ O2/.4/ B2CO/.75/ CO2/1.5/ H2O/6.5/ CH4/.48/  
     HE/0.35/ C2H4Z/1.6/ AR/.24/  
 B6CH2+R1H=B4CH+H2                    3.0E13            0.            0.            !(4,-  
 4)<TSANG86>!  
  
 !REACTIONS DE B5CH2!  
 B5CH2+R1H=B4CH+H2                    6.0E12            0.            -1.8E3        !(5,-  
 5)<BAULCH94>!  
 B5CH2+B3C=R9C2HT+R1H                5.0E13            0.            0.            !(6,-  
 6)<RANZI94>!  
 B5CH2+B5CH2=>C2H2T+R1H+R1H        1.2E14            0.            0.8E3        !(7)<BAULCH94>!  
  
 !REACTIONS DE R4CH3!  
 R4CH3+M=B5CH2+R1H+M                2.91E16            0.0            90.7E3        !(8,-  
 8)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
 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=C2H2T+R1H                   5.0E13            0.            0.            !(13,-  
 13)<RANZI94>!  
 R4CH3+R4CH3 (+M) =>C2H6 (+M)        3.61E13            0.            0.            !(14)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
     LOW / 3.63E41    -7.0    2.76E3 /  
     TROE / 0.62    73    1180 /  
 C2H6 (+M) =>R4CH3+R4CH3 (+M)        1.8E21            -1.24        90.9E3        !(-  
 14)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
     LOW / 1.89E49    -8.24    93.7E3/  
     TROE / 0.62    73    1180 /  
 R4CH3+R4CH3=R11C2H5+R1H             3.0E13            0.            13.5E3        !(15,-  
 15)<BAULCH94>!  
 R4CH3+R4CH3=C2H4Z+H2                2.1E14            0.            19.3E3        !(16,-  
 16)<FRANK86NIST>!  
  
 !REACTIONS DE CH4!  
 R1H+R4CH3 (+M) =>CH4 (+M)            1.67E14            0.            0.            !(17)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
     LOW / 1.408E24    -1.8    0.0 /  
     TROE / 0.37    3315    61 /  
 CH4 (+M) =>R4CH3+R1H (+M)            2.4E16            0.            105.0E3        !(-  
 17)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/



N2/0.4/ HE/0.35/  
 LOW / 1.29E18 0.00 90.9E3 /  
 TROE / 0 1350 1 7830 /  
 CH4(+CH4)=>R4CH3+R1H(+CH4) 2.4E16 0. 105.0E3 !(-  
 17')<BAULCH94>!  
 LOW / 8.43E17 0.00 90.9E3 /  
 TROE / 0.69 90 2210 /  
 CH4+R1H=R4CH3+H2 1.3E04 3. 8.0E3 !(18,-  
 18)<BAULCH94>!  
 CH4+B4CH=C2H4Z+R1H 3.0E13 0. -0.4E3 !(19,-  
 19)<DAGAUT91BAULCH94>!  
 CH4+B6CH2=R4CH3+R4CH3 4.2E13 0. 0. !(20,-  
 20)<TSANG86>!  
  
 !REACTIONS DE R9C2HT!  
 R9C2HT+B6CH2=C2H2T+B4CH 1.8E13 0. 0. !(21,-  
 21)<TSANG86>!  
 R9C2HT+B5CH2=C2H2T+B4CH 1.8E13 0. 0. !(22,-  
 22)<TSANG86>!  
 R9C2HT+CH4=C2H2T+R4CH3 1.2E12 0. 0. !(23,-  
 23)<BAULCH94>!  
  
 !REACTIONS DE C2H2T!  
 C2H2T+M=R9C2HT+R1H+M 1.14E17 0. 107.0E3 !(24,-  
 24)<BAULCH94>!  
 O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 N2/0.4/ HE/0.35/  
 C2H2T+R1H=R9C2HT+H2 6.6E13 0. 27.7E3 !(25,-  
 25)<BAULCH94>!  
  
 !REACTIONS DE R10C2H3V!  
 R10C2H3V(+M)=C2H2T+R1H(+M) 2.0E14 0. 39.8E3 !(26,-  
 26)<BAULCH94>!  
 O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ AR/0.35/  
 N2/0.4/ HE/0.35/  
 LOW / 1.19E42 -7.50 45.55E3 /  
 TROE /0.35 1.0 1.E8/  
 R10C2H3V+R1H=C2H2T+H2 1.2E13 0. 0. !(27,-  
 27)<BAULCH94>!  
 R10C2H3V+B6CH2=C2H2T+R4CH3 1.8E13 0. 0. !(28,-  
 28)<TSANG86>!  
 R10C2H3V+B5CH2=C2H2T+R4CH3 1.8E13 0. 0. !(29,-  
 29)<TSANG86>!  
 R10C2H3V+R4CH3=CH4+C2H2T 3.9E11 0. 0. !(30,-  
 30)<TSANG86>!  
 R10C2H3V+R9C2HT=2C2H2T 9.6E11 0. 0. !(31,-  
 31)<TSANG86>!  
 R10C2H3V+R10C2H3V=C2H4Z+C2H2T 9.6E11 0. 0. !(32,-  
 32)<TSANG86>!  
  
 !REACTIONS DE C2H4Z!  
 C2H4Z+M=C2H2T+H2+M 9.97E16 0. 71.6E3 !(33,-  
 33)<BAULCH94>!  
 O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 N2/0.4/ HE/0.35/  
 C2H4Z+M=R10C2H3V+R1H+M 7.40E17 0. 96.7E3 !(34,-  
 34)<BAULCH94>!  
 O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/

N2/0.4/ HE/0.35/  
 C2H4Z+R1H=R10C2H3V+H2 5.0E7 1.93 13.0E3 !(35,-  
 35) SLAGLE96!  
 C2H4Z+R4CH3=CH4+R10C2H3V 6.3E11 0. 16.0E3 !(36,-36) BACK89!

!REACTIONS DE R11C2H5!  
 R11C2H5(+M)=C2H4Z+R1H(+M) 8.2E13 0. 40.0E3 !(37,-37)  
 BAULCH94!  
 O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 N2/0.4/ HE/0.35/  
 LOW / 3.40E17 0.00 33.4E3 /  
 TROE / 0.75 97 1379/

R11C2H5+R1H=C2H4Z+H2 1.8E12 0. 0. !(38,-  
 38)<TSANG86>!  
 R11C2H5+R1H=C2H6 3.6E13 0. 0. !(39,-  
 39)<TSANG86>!  
 R11C2H5+B6CH2=C2H4Z+R4CH3 9.0E12 0. 0. !(40,-  
 40)<TSANG86>!  
 R11C2H5+B5CH2=C2H4Z+R4CH3 1.8E13 0. 0. !(41,-  
 41)<TSANG86>!  
 R11C2H5+R4CH3=C2H4Z+CH4 1.1E12 0. 0. !(42,-  
 42)<BAULCH94>!  
 R11C2H5+R9C2HT=C2H2T+C2H4Z 1.8E12 0. 0. !(43,-  
 43)<TSANG86>!  
 R11C2H5+R10C2H3V=2C2H4Z 4.8E11 0. 0. !(44,-  
 44)<TSANG86>!  
 R11C2H5+R10C2H3V=C2H2T+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+R9C2HT=C2H2T+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 53) <BAULCH94>!	5.1E4	2.67	6.2E3	!(53,-
B1O+B4CH=B2CO+R1H 54) <BAULCH94>!	3.9E13	0.	0.	!(54,-
B1O+B4CH=B3C+R2OH 55) <MUR86NIS>!	1.5E13	0.	4.7E3	!(55,-
B1O+B6CH2=>B2CO+2R1H <TSANG86>!	1.5E13	0.	0.	!(56)
B1O+B6CH2=B2CO+H2 <TSANG86>!	1.5E13	0.	0.	!(57,-57)
B1O+B5CH2=>B2CO+2R1H <BAULCH94>!	7.2E13	0.	0.	!(58)
B1O+B5CH2=B2CO+H2 59) <BAULCH94>!	4.8E13	0.	0.	!(59,-
B1O+R4CH3=HCHO+R1H 60) <BAULCH94>!	8.4E13	0.	0.	!(60,-
B1O+R4CH3=R7CH3O 61) <DEAN87NIS>!	8.0E15	-2.12	0.6E3	!(61,-
B1O+CH4=R4CH3+R2OH 62) <BAULCH94>!	7.2E8	1.56	8.4E3	!(62,-
B1O+R9C2HT=B4CH+B2CO 63) <DAGAUT91>!	1.0E13	0.	0.	!(63,-
B1O+C2H2T=B5CH2+B2CO LEEDS>!	2.17E06	2.1	1.6E3	!(64,-64) <BAULCH
B1O+C2H2T=R12CHCOV+R1H LEEDS>!	5.06E06	2.1	1.6E3	!(65,-65) <BAULCH
B1O+R10C2H3V=R4CH3+B2CO 66) <DAGAUT91>!	3.0E13	0.	0.	!(66,-
B1O+R10C2H3V=CH2COZ+R1H 67) <TSANG86>!	9.6E13	0.	0.	!(67,-
B1O+C2H4Z=R4CH3+R5CHO 68) <BAULCH94>!	8.1E6	1.88	0.2E3	!(68,-
B1O+C2H4Z=HCHO+B5CH2 69) <BAULCH94>!	4.00E5	1.88	0.2E3	!(69,-
B1O+C2H4Z=CH2COZ+H2 70) <BAULCH94>!	6.6E5	1.88	0.2E3	!(70,-
B1O+C2H4Z=R13CH2CHO+R1H 71) <BAULCH94>!	4.7E6	1.88	0.2E3	!(71,-
B1O+C2H4Z=R2OH+R10C2H3V 72) <MAHMUD87NIST>!	1.5E7	1.91	3.7E3	!(72,-
B1O+R11C2H5=HCHO+R4CH3 73) <BAULCH94>!	1.1E13	0.	0.	!(73,-
B1O+R11C2H5=CH3CHO+R1H 74) <BAULCH94>!	5.5e13	0.	0.	!(74,-
B1O+R11C2H5=C2H4Z+R2OH 75) <DAGAUT91>!	3.0E13	0.	0.	!(75,-
B1O+C2H6=R11C2H5+R2OH 76) <BAULCH94>!	1.0E9	1.5	5.8E3	!(76,-

!REACTIONS DE R2OH!

R1H+B1O+M=R2OH+M 77) <BAULCH94>!	1.18E19	-1.0	0.0	!(77,-
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/				
R1H+R2OH+M=H2O+M 78) <BAULCH94>!	5.53E+22	-2.0	0.0	!(78,-
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/ N2/0.4/ HE/0.35/				

R2OH+H2=R1H+H2O 79) <BAULCH94>!	1.0E8	1.6	3.3E3	!(79,-
R2OH+B3C=B2CO+R1H 80) <RANZI94>!	5.0E13	0.	0.	!(80,-
R2OH+B4CH=R5CHO+R1H 81) <DAGAUT91>!	3.0E13	0.	0.	!(81,-
R2OH+B6CH2=HCHO+R1H 82) <TSANG86>!	3.0E13	0.	0.	!(82,-
R2OH+B5CH2=HCHO+R1H 83) <TSANG86>!	1.8E13	0.	0.	!(83,-
R2OH+R4CH3=B6CH2+H2O 84) <BAULCH94>!	7.2E13	0.	2.7E3	!(84,-
R2OH+R4CH3 (+M)=CH3OH (+M) 85) <BAULCH94>!	6.0E13	0.	0.	!(85,-
LOW /1.4E44	-8.2	0./		
TROE /0.82	200.	1438./		
R2OH+R4CH3=HCHO+H2 86) <DAGAUT91>!	3.2E12	-0.53	10.8E3	!(86,-
R2OH+R4CH3=R7CH3O+R1H 87) <DAGAUT91>!	5.7E12	-0.23	13.9E3	!(87,-
R2OH+CH4=R4CH3+H2O 88) <BAULCH94>!	1.6E7	1.83	2.7E3	!(88,-
R2OH+R9C2HT=C2H2T+B1O 89) <TSANG86>!	1.8E13	0.	0.	!(89,-
R2OH+R9C2HT=B5CH2+B2CO 90) <TSANG86>!	1.8E13	0.	0.	!(90,-
R2OH+R9C2HT=R12CHCOV+R1H 91) <DAGAUT91>!	2.0E13	0.	0.	!(91,-
R2OH+C2H2T=R9C2HT+H2O 92) <TSANG86>!	1.4E4	2.68	12.0E3	!(92,-
R2OH+C2H2T=CH2COZ+R1H 93) <DAGAUT91>!	2.2E-4	4.5	-1.0E3	!(93,-
R2OH+C2H2T=R4CH3+B2CO 94) <DAGAUT91>!	4.8E-4	4.	-2.0E3	!(94,-
R2OH+R10C2H3V=C2H2T+H2O 95) <TSANG86>!	3.0E13	0.	0.	!(95,-
R2OH+R10C2H3V=CH3CHO 96) <TSANG86>!	3.0E13	0.	0.	!(96,-
R2OH+C2H4Z=R10C2H3V+H2O 97) <BAULCH94>!	2.0E13	0.	5.9E3	!(97,-
R2OH+C2H4Z=R4CH3+HCHO 98) <GLARBORG86>!	2.0E12	0.	0.9E3	!(98,-
R2OH+R11C2H5=C2H4Z+H2O 99) <TSANG86>!	2.4E13	0.	0.	!(99,-
R2OH+R11C2H5=>R4CH3+R1H+HCHO <TSANG86>!	2.4E13	0.	0.	!(100)
R2OH+C2H6=R11C2H5+H2O 101) <BAULCH94>!	7.2E6	2.	0.9E3	!(101,-
R2OH+R2OH=H2O+B1O 102) <BAULCH94>!	1.5E9	1.14	0.1E3	!(102,-
!REACTIONS DE H2O!				
H2O+B4CH=R6CH2OH 103) <BAULCH94>!	5.7E12	0.	-0.8E3	!(103,-
H2O+B6CH2=CH3OH 104) <TSANG86>!	1.8E13	0.	0.	!(104,-

!REACTIONS DE B2CO!

B2CO+R4CH3 (+M)=R14CH3CO (+M) 5.0E11 0. 6.9E3 !(105,-  
 105)<BAULCH94>!  
     LOW /1.1E14 0. 3.8E3/  
     TROE /0.5 1.0 1.0E8/  
 B2CO+B1O+M=CO2+M 1.54E15 0.0 3.0E3 !(106,-  
 106)<TSANG86>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
 B2CO+R2OH=CO2+R1H 6.3E6 1.5 -0.5E3 !(107,-  
 107)<BAULCH94>!  
  
 !REACTIONS DE R5CHO!  
 R5CHO+M=R1H+B2CO+M 1.9E17 -1. 17.0E3 !(108,-  
 108)<WANG97>!  
     H2/2.0/ B2CO/1.5/ CO2/2.0/ H2O/6.0/  
 R5CHO+R1H=H2+B2CO 9.0E13 0. 0. !(109,-  
 109)<BAULCH94>!  
 R5CHO+R1H=B1O+B5CH2 4.0E13 0. 102.5E3 !(110,-  
 110)<TSUBOI81NIST>!  
 R5CHO+B6CH2=R4CH3+B2CO 1.8E13 0. 0. !(111,-  
 111)<TSANG86>!  
 R5CHO+B5CH2=R4CH3+B2CO 1.8E13 0. 0. !(112,-  
 112)<TSANG86>!  
 R5CHO+R4CH3=CH4+B2CO 1.2E14 0. 0. !(113,-  
 113)<TSANG86>!  
 R5CHO+R4CH3=CH3CHO 1.8E13 0. 0. !(114,-  
 114)<TSANG86>!  
 R4CH3+HCHO=R5CHO+CH4 7.7E-8 6.1 1.97E3 !(115,-  
 115)<BAULCH94>!  
 R5CHO+R9C2HT=C2H2T+B2CO 6.0E13 0. 0. !(116,-  
 116)<TSANG86>!  
 R5CHO+R10C2H3V=C2H4Z+B2CO 9.0E13 0. 0. !(117,-  
 117)<TSANG86>!  
 R10C2H3V+HCHO=R5CHO+C2H4Z 5.4E3 2.81 5.9E3 !(118,-  
 118)<TSANG86>!  
 R5CHO+R11C2H5=C2H6+B2CO 1.2E14 0. 0. !(119,-  
 119)<TSANG86>!  
 R11C2H5+HCHO=R5CHO+C2H6 5.57E3 2.81 5.86E3 !(120,-  
 120)<TSANG86>!  
 R5CHO+B1O=R1H+CO2 3.0E13 0. 0. !(121,-  
 121)<BAULCH94>!  
 R5CHO+B1O=R2OH+B2CO 3.0E13 0. 0. !(122,-  
 122)<BAULCH94>!  
 R5CHO+R2OH=H2O+B2CO 1.1E14 0. 0. !(123,-  
 123)<BAULCH94>!  
 R5CHO+R5CHO=HCHO+B2CO 3.0E13 0. 0. !(124,-  
 124)<BAULCH94>!  
  
 !REACTIONS DE HCHO!  
 HCHO+M=R5CHO+R1H+M 1.40E36 -5.54 96.8E3 !(125,-  
 125)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/  
 HCHO+M=H2+B2CO+M 3.26E36 -5.54 96.8E3 !(126,-  
 126)<BAULCH94>!  
     O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
     N2/0.4/ HE/0.35/

HCHO+R1H=R5CHO+H2	1.3E8	1.62	2.1E3	!(127,-
127)<BAULCH94>!				
HCHO+B4CH=R13CH2CHO	9.6E13	0.	-0.5E3	!(128,-
128)<BAULCH94average>!				
HCHO+B6CH2=R4CH3+R5CHO	1.2E12	0.	0.	!(129,-
129)<TSANG86>!				
HCHO+B1O=R5CHO+R2OH	4.1E11	0.57	2.7E3	!(130,-
130)<BAULCH94>!				
HCHO+R2OH=R5CHO+H2O	7.82E7	1.63	-1.06E3	!(131,-
131)<BAULCH94> ; nouvelles données M. Cord !				

!REACTIONS DE R7CH3O!

R7CH3O+M=HCHO+R1H+M	1.55E14	0.00	13.5E3	!(132,-
132)<BAULCH94>!				
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/				
R7CH3O+R1H=HCHO+H2	1.8E13	0.	0.	!(133,-
133)<BAULCH94>!				
R7CH3O+B6CH2=R4CH3+HCHO	1.8E13	0.	0.	!(134,-
134)<TSANG86>!				
R7CH3O+B5CH2=R4CH3+HCHO	1.8E13	0.	0.	!(135,-
135)<TSANG86>!				
R7CH3O+R4CH3=HCHO+CH4	2.4E13	0.	0.	!(136,-
136)<TSANG86>!				
R7CH3O+CH4=R4CH3+CH3OH	1.6E11	0.	8.8E3	!(137,-
137)<TSANG86>!				
R7CH3O+R9C2HT=HCHO+C2H2T	2.4E13	0.	0.	!(138,-
138)<TSANG86>!				
R7CH3O+R10C2H3V=HCHO+C2H4Z	2.4E13	0.	0.	!(139,-
139)<TSANG86>!				
R7CH3O+C2H4Z=HCHO+R11C2H5	1.2E11	0.	6.7E3	!(140,-
140)<TSANG86>!				
R7CH3O+R11C2H5=HCHO+C2H6	2.4E13	0.	0.	!(141,-
141)<TSANG86>!				
R7CH3O+C2H6=R11C2H5+CH3OH	2.4E11	0.	7.0E3	!(142,-
142)<TSANG86>!				
R7CH3O+B1O=HCHO+R2OH	1.8E12	0.	0.	!(143,-
143)<BAULCH94>!				
R7CH3O+R2OH=HCHO+H2O	1.8E13	0.	0.	!(144,-
144)<TSANG86>!				
R7CH3O+B2CO=R4CH3+CO2	1.6E13	0.	11.7E3	!(145,-
145)<TSANG86>!				
R7CH3O+R5CHO=CH3OH+B2CO	9.1E13	0.	0.	!(146,-
146)<TSANG86>!				
R7CH3O+HCHO=CH3OH+R5CHO	1.0E11	0.	3.0E3	!(147,-
147)<TSANG86>!				
R7CH3O+R7CH3O=CH3OH+HCHO	6.0E13	0.	0.	!(148,-
148)<TSANG86>!				

!REACTIONS DE R6CH2OH!

R6CH2OH+M=HCHO+R1H+M	1.26E16	0.00	30.0E3	!(149,-
149)<BAULCH>!				
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/				
R6CH2OH+R1H=R4CH3+R2OH	9.6E13	0.	0.	!(150,-
150)<TSANG87>!				
R6CH2OH+R1H=HCHO+H2	6.0E12	0.	0.	!(151,-
151)<TSANG87>!				

R6CH2OH+H2=CH3OH+R1H 152)<TSANG87>!	6.7E5	2.	13.4E3	!(152,-
R6CH2OH+B6CH2=CH3CHO+R1H 153)<TSANG87>!	1.8E13	0.	0.	!(153,-
R6CH2OH+B5CH2=C2H4Z+R2OH 154)<TSANG87>!	2.4E13	0.	0.	!(154,-
R6CH2OH+B5CH2=R4CH3+HCHO 155)<TSANG87>!	1.2E12	0.	0.	!(155,-
R6CH2OH+R4CH3=C2H5OH 156)<TSANG87>!	1.2E13	0.	0.	!(156,-
R6CH2OH+R4CH3=CH4+HCHO 157)<TSANG87>!	2.4E12	0.	0.	!(157,-
R6CH2OH+CH4=CH3OH+R4CH3 158)<TSANG87>!	21.7	3.1	16.2E3	!(158,-
R6CH2OH+R9C2HT=C2H2T+HCHO 159)<TSANG87>!	4.8E13	0.	0.	!(159,-
!la constante de vitesse du processus 159 est globalisee!				
!R6CH2OH+R9C2HT=C3H3+R2OH 159a)<TSANG87>!	1.2E13	0.	0.	!(159a,-
!R6CH2OH+R9C2HT=C2H2T+HCHO 159b)<TSANG87>!	3.6E13	0.	0.	!(159b,-
R6CH2OH+C2H2T=R10C2H3V+HCHO 160)<TSANG87>!	7.2E11	0.	9.0E3	!(160,-
R6CH2OH+R10C2H3V=C2H4Z+HCHO 161)<TSANG87>!	4.2E13	0.	0.	!(161,-
!La constante de vitesse du processus 161 est globalisee!				
R6CH2OH+R11C2H5=C2H4Z+CH3OH 162)<TSANG87>!	2.4E12	0.	0.	!(162,-
R6CH2OH+R11C2H5=C2H6+HCHO 163)<TSANG87>!	2.4E12	0.	0.	!(163,-
R6CH2OH+C2H6=CH3OH+R11C2H5 164)<TSANG87>!	199.	3.	14.0E3	!(164,-
R6CH2OH+B1O=HCHO+R2OH 165)<TSANG87>!	4.2E13	0.	0.	!(165,-
R6CH2OH+R2OH=H2O+HCHO 166)<TSANG87>!	2.4E13	0.	0.	!(166,-
R6CH2OH+R5CHO=CH3OH+B2CO 168)<TSANG87>!	1.2E14	0.	0.	!(168,-
R6CH2OH+R5CHO=HCHO+HCHO 169)<TSANG87>!	1.8E14	0.	0.	!(169,-
R6CH2OH+HCHO=CH3OH+R5CHO 170)<TSANG87>!	5.5E3	2.8	5.9E3	!(170,-
R6CH2OH+R7CH3O=CH3OH+HCHO 171)<TSANG87>!	2.4E13	0.	0.	!(171,-
R6CH2OH+R6CH2OH=CH3OH+HCHO 172)<TSANG87>!	1.4E13	0.	0.	!(172,-
!la constante de vitesse du processus 172 est globalisee!				
!R6CH2OH+R6CH2OH=CH3OH+HCHO 172a)<TSANG87>!	4.8E12	0.	0.	!(172a,-
!R6CH2OH+R6CH2OH=HOCH2CH2OH 172b)<TSANG87>!	9.6E12	0.	0.	!(172b,-
!REACTIONS DE CH3OH!				
CH3OH+R1H=R4CH3+H2O 173)<HIDAKA89NIST>!	2.0E14	0.	5.3E3	!(173,-
CH3OH+R1H=R7CH3O+H2 174)<TSANG87>!	4.2E6	2.1	4.9E3	!(174,-

CH3OH+B6CH2=R6CH2OH+R4CH3 175) <TSANG87>!	1.5E12	0.	0. ! (175,-
CH3OH+B5CH2=R4CH3+R6CH2OH 176) <TSANG87>!	31.9	3.2	7.2E3 ! (176,-
CH3OH+B5CH2=R4CH3+R7CH3O 177) <TSANG87>!	14.4	3.1	6.9E3 ! (177,-
CH3OH+R9C2HT=C2H2T+R6CH2OH 178) <TSANG87>!	6.0E12	0.	0. ! (178,-
CH3OH+R9C2HT=C2H2T+R7CH3O 179) <TSANG87>!	1.2E12	0.	0. ! (179,-
CH3OH+R10C2H3V=C2H4Z+R6CH2OH 180) <TSANG87>!	31.9	3.2	7.2E3 ! (180,-
CH3OH+R10C2H3V=C2H4Z+R7CH3O 181) <TSANG87>!	14.4	3.1	6.9E3 ! (181,-
CH3OH+B1O=R6CH2OH+R2OH 182) <GROTHER81NIST>!	3.4E13	0.	5.5E3 ! (182,-
CH3OH+B1O=R7CH3O+R2OH 183) <WARNATZ84>!	1.0E13	0.	4.7E3 ! (183,-
CH3OH+R2OH=R6CH2OH+H2O 184a) <Atkinson86>85%!	3.1E06	2.	-3.4E2 ! (184a,-
CH3OH+R2OH=R7CH3O+H2O 184b) <Atkinson86>15%!	5.4E05	2.	-3.4E2 ! (184b,-
CH3OH+R7CH3O=CH3OH+R6CH2OH 185) <TSANG87>!	3.0E11	0.	4.1E3 ! (185,-

!REACTIONS DE R12CHCOVD!

R12CHCOV+M=B4CH+B2CO+M 186) <DAGAUT91>!	6.0E15	0.	58.8E3 ! (186,-
R12CHCOV+R1H=B5CH2+B2CO 187a) <BAULCH94>!	1.5E14	0.	0. ! (187a,-
R12CHCOV+R1H=B6CH2+B2CO 187b) <PEETERS97>!	1.3E14	0.	0. ! (187b,-
R12CHCOV+B5CH2=R9C2HT+HCHO 188) <DAGAUT91>!	1.0E13	0.	2.0E3 ! (188,-
R12CHCOV+B5CH2=R10C2H3V+B2CO 189) <DAGAUT91>!	3.0E13	0.	0. ! (189,-
R12CHCOV+B1O=>B2CO+B2CO+R1H ! (190) <BAULCH94>!	9.6E13	0.	0.
R12CHCOV+R2OH=>R5CHO+B2CO+R1H ! (191) <DAGAUT91>!	1.0E13	0.	0.

!REACTIONS DE CH2COZD!

CH2COZ+M=B6CH2+B2CO+M 192) <FRANK86NIST>! O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/	6.57E15	0.0	57.6E3 ! (192,-
CH2COZ+M=R12CHCOV+R1H+M 193) <FRANK86NIST>! O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/	2.7E17	0.	87.0E3 ! (193,-
CH2COZ+R1H=R4CH3+B2CO 194) <BAULCH94>!	1.8E13	0.	3.4E3 ! (194,-
CH2COZ+R1H=R12CHCOV+H2 195) <DAGAUT91>!	5.0E13	0.	8.0E3 ! (195,-
CH2COZ+B5CH2=C2H4Z+B2CO 196) <CANOSA-MAS84NIST>!	1.3E14	0.	0. ! (196,-



CH2COZ+B1O=B5CH2+CO2 197) <DAGAUT91>!	1.8E12	0.	1.3E3 ! (197,-
CH2COZ+B1O=R12CHCOV+R2OH 198) <DAGAUT91>!	1.0E13	0.	8.0E3 ! (198,-
CH2COZ+R2OH=R12CHCOV+H2O 199) <DAGAUT91>!	7.5E12	0.	2.0E3 ! (199,-
CH2COZ+R2OH=R4CH3+CO2 200a) <BAULCH LEEDS>!	2.52E12	0.	0. ! (200a,-
CH2COZ+R2OH=R6CH2OH+B2CO 200b) <BAULCH LEEDS>!	4.68E12	0.	0. ! (200b,-

!REACTIONS DE R14CH3CO!

R14CH3CO+R1H=R4CH3+R5CHO 201) <TSANG86>!	9.6E13	0.	0. ! (201,-
R14CH3CO+B6CH2=R4CH3+CH2COZ 202) <TSANG86>!	1.8E13	0.	0. ! (202,-
R14CH3CO+B5CH2=R4CH3+CH2COZ 203) <TSANG86>!	1.8E13	0.	0. ! (203,-
R14CH3CO+B1O=R4CH3+CO2 204) <TSANG86>!	9.6E12	0.	0. ! (204,-
R14CH3CO+R2OH=CH2COZ+H2O 205) <TSANG86>!	1.2E13	0.	0. ! (205,-
R14CH3CO+R2OH=>R4CH3+B2CO+R2OH ! (206) <TSANG86>!	3.0E13	0.	0.
R14CH3CO+R5CHO=CH3CHO+B2CO 207) <TSANG86>!	9.0E12	0.	0. ! (207,-
R14CH3CO+HCHO=CH3CHO+R5CHO 208) <TSANG86>!	1.8E11	0.	12.9E3! (208,-
R14CH3CO+R7CH3O=CH3OH+CH2COZ 209) <TSANG86>!	6.0E12	0.	0. ! (209,-
R14CH3CO+R7CH3O=HCHO+CH3CHO 210) <TSANG86>!	6.0E12	0.	0. ! (210,-
R14CH3CO+CH3OH=CH3CHO+R6CH2OH 211) <TSANG87>!	4.85E3	3.	12.3E3! (211,-
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 212) <TSANG86>!	1.2E13	0.	0. ! (212,-

!REACTIONS DE R13CH2CHO!

R13CH2CHO=R14CH3CO 213) <COLKET75NIST>!	1.0E13	0.	47.0E3! (213,-
R13CH2CHO=R1H+CH2COZ 214) <COLKET75NIST>!	1.6E13	0.	35.0E3! (214,-

!REACTIONS DE CH3CHO!

CH3CHO+R1H=H2+R14CH3CO 215) <WARNATZ84>!	4.0E13	0.	4.2E3 ! (215,-
CH3CHO+R4CH3=R14CH3CO+CH4 216) <BAULCH94>!	2.0E-6	5.6	2.5E3 ! (216,-
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO 217) <SCHERZER87>!	8.1E10	0.	3.7E3 ! (217,-
CH3CHO+R11C2H5=C2H6+R14CH3CO 218) <HOHLEIN70>!	1.3E12	0.	8.5E3 ! (218,-
CH3CHO+B1O=R14CH3CO+R2OH 219) <CAVANAGH90>!	1.4E13	0.	2.3E3 ! (219,-
CH3CHO+R2OH=R14CH3CO+H2O 220) <CAVANAGH90>!	4.2E12	0.	0.5E3 ! (220,-

CH3CHO+R7CH3O=R14CH3CO+CH3OH 2.4E11 0. 1.8E3 !(221,-  
 221) <CAVANAGH90>!  
 CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 2.5E7 0. 0. !(222,-  
 222) <SCHUCHMANN70NIST>!

!REACTIONS DE C2H4O#1

C2H4OE#3=CH4+B2CO 1.2E13 0. 57.2E3 !(223,-  
 223) <LIFSHITZ83NIST>!  
 C2H4OE#3=CH3CHO 7.3E13 0. 57.2E3 !(224,-  
 224) <LIFSHITZ83NIST>!  
 C2H4OE#3=R4CH3+R5CHO 3.6E13 0. 57.2E3 !(225,-  
 225) <LIFSHITZ83NIST>!  
 C2H4OE#3+R1H=H2+R13CH2CHO 2.0E13 0. 8.3E3 !(226,-  
 226) <LIFSHITZ83NIST\*>!  
 C2H4OE#3+R1H=H2O+R10C2H3V 5.0E9 0. 5.0E3 !(227,-  
 227) <LIFSHITZ83NIST>!  
 C2H4OE#3+R1H=C2H4Z+R2OH 9.5E10 0. 5.0E3 !(228,-  
 228) <LIFSHITZ83NIST>!  
 C2H4OE#3+R4CH3=CH4+R13CH2CHO 1.1E12 0. 11.8E3 !(229,-  
 229) <BALDWIN84NIST\*>!  
 C2H4OE#3+R4CH3=R11C2H5+HCHO 1.4E11 0. 7.6E3 !(230,-  
 230) <RANZI94>!  
 C2H4OE#3+R4CH3=C2H4Z+R7CH3O 1.5E10 0. 7.6E3 !(231,-  
 231) <RANZI94>!  
 C2H4OE#3+R9C2HT=C2H2T+R13CH2CHO 1.2E12 0. 9.8E3 !(232,-  
 232) <RANZI94>!  
 C2H4OE#3+R10C2H3V=C2H4Z+R13CH2CHO 2.0E12 0. 9.3E3 !(233,-  
 233) <RANZI94>!  
 C2H4OE#3+R11C2H5=C2H6+R13CH2CHO 6.8E11 0. 11.4E3 !(234,-  
 234) <RANZI94>!  
 C2H4OE#3+B1O=R2OH+R13CH2CHO 1.9E12 0. 5.2E3 !(235,-  
 235) <BOGAN78NIST>!  
 C2H4OE#3+R2OH=H2O+R13CH2CHO 1.8E13 0. 3.6E3 !(236,-  
 236) <BALDWIN84NIST\*>!  
 C2H4OE#3+R5CHO=HCHO+R13CH2CHO 3.7E12 0. 15.8E3 !(237,-  
 237) <RANZI94>!  
 C2H4OE#3+R7CH3O=CH3OH+R13CH2CHO 1.3E12 0. 5.8E3 !(238,-  
 238) <RANZI94>!  
 C2H4OE#3+R6CH2OH=CH3OH+R13CH2CHO 8.4E11 0. 13.4E3 !(239,-  
 239) <RANZI94>!  
 C2H4OE#3+R14CH3CO=CH3CHO+R13CH2CHO 4.0E12 0. 17.5E3 !(240,-  
 240) <RANZI94>!  
 C2H4OE#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>!

!Réactions de la base alcool

! bêta-scissions:

C2H4Z+R2OH(+M)=R24C2H4OH(+M) 5.420E+12 0.0 0.0  
 LOW / 1.19E27 -3.1 0.0 /

R24C2H4OH=R1H+CH3CHO	3.000E+13	0.0	34800.0	
R25C2H4OH=CH3CHO+R1H	3.000E+13	0.0	38000.0	! 3H
primaire				
R25C2H4OH+M=CH3CHO+R1H+M	5.000E+13	0.0	21860.0	
! Konnov				
! isomérisation :				
R24C2H4OH=R25C2H4OH	1.000E+11	0.0	27000.0	!
Konnov				
!oxydations :				
R24C2H4OH+O2=CH3CHO+R3OOH	1.600E+12	0.0	5000.0	
R25C2H4OH+O2=CH3CHO+R3OOH	8.400E+15	-1.20	0.0	!
Konnov				
DUPLICATE				
R25C2H4OH+O2=CH3CHO+R3OOH	4.800E+14	0.0	5000.0	
! Konnov				
DUPLICATE				
R25C2H4OH+R1H=CH3CHO+H2	2.000E+13	0.0	0.0	
R25C2H4OH+R2OH=CH3CHO+H2O	1.500E+13	0.0	0.0	
R25C2H4OH+B1O=CH3CHO+R2OH	9.040E+13	0.0	0.0	
!!!!!! Réactions de l'éthanol (à substituer aux réactions de l'éthanol dans la base C0-C2)				
!Amorçage bimoléculaire de l'éthanol				
C2H5OH+O2=R24C2H4OH+R3OOH	4.000E+13	0.0	50900.0	
C2H5OH+O2=R25C2H4OH+R3OOH	4.000E+13	0.0	51200.0	
!Métathèse de l'éthanol C2H5OH				
C2H5OH+R2OH=R24C2H4OH+H2O	2.563E+06	2.06	860.0	
C2H5OH+R2OH=R25C2H4OH+H2O	3.000E+13	0.0	5960.0	
C2H5OH+B1O=R25C2H4OH+R2OH	6.000E+05	2.46	1850.0	
C2H5OH+B1O=R24C2H4OH+R2OH	5.000E+12	0.0	4411.0	
C2H5OH+R1H=R25C2H4OH+H2	4.400E+12	0.0	4570.0	
C2H5OH+R3OOH=R25C2H4OH+H2O2	2.000E+13	0.0	17000.0	
C2H5OH+R4CH3=R25C2H4OH+CH4	4.000E+11	0.0	9700.0	
C2H5OH+R4CH3=R24C2H4OH+CH4	3.000E+00	4.0	10480.0	
C2H5OH+R1H=R24C2H4OH+H2	2.000E+12	0.0	9500.0	
C2H5OH+R11C2H5=R24C2H4OH+C2H6	1.500E+12	0.0	11700.0	
C2H5OH+R11C2H5=R25C2H4OH+C2H6	4.000E+13	0.0	10000.0	
C2H5OH+R6CH2OH=R25C2H4OH+CH3OH	4.000E+11	0.0	9700.0	
C2H5OH+R7CH3O=R25C2H4OH+CH3OH	2.000E+11	0.0	7000.0	
C2H5OH+R15C2H5O=C2H5OH+R25C2H4OH	2.000E+11	0.0	7000.0	
!REACTIONS DE O2!				
B1O+B1O+M=O2+M	5.40E13	0.	-1.79E3	!(244,-
244)<BAULCH94>!				
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
N2/0.4/ HE/0.35/				
O2+R1H=R2OH+B1O	9.8E13	0.	14.8E3	!(245,-
245)<BAULCH94>!				

O2+R1H (+M)=R3OOH (+M) 246) <COBOS85>!	4.52E13	0.	0.	!(246,-
LOW /1.8E18	-0.8	0.00/	!k0 BAULCH94!	
TROE /0.5	1.0	1.0E8/		
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/ HE/0.35/ N2/0.67/				
O2+R1H (+H2O)=R3OOH (+H2O) 246b) <BAULCH94>!	4.52E13	0.	0.	!(246b,-
LOW /6.9E15	0.0	-2080/		
TROE /0.45	1.0	1.0E8/		
O2+B3C=B2CO+B1O 247) <RANZI94>!	1.2E14	0.	0.	!(247,-
O2+B4CH=R5CHO+B1O 248) <DAGAUT91>!	3.3E13	0.	0.	!(248,-
O2+B4CH=B2CO+R2OH 249) <PEETERS97>!	3.2E13	0.	0.	!(249,-
O2+B6CH2=>B2CO+R2OH+R1H !(250) <BAULCH94>!	3.1E12	0.	0.	
O2+B5CH2=R5CHO+R2OH 251) <DAGAUT91>!	4.3E10	0.	-0.5E3	!(251,-
O2+B5CH2=CO2+H2 252) <DAGAUT91>!	6.9E11	0.	0.5E3	!(252,-
O2+B5CH2=>CO2+R1H+R1H !(253) <DAGAUT91>!	1.6E12	0.	1.0E3	
O2+B5CH2=B2CO+H2O 254) <DAGAUT91>!	1.9E10	0.	-1.0E3	!(254,-
O2+B5CH2=>B2CO+R2OH+R1H !(255) <DAGAUT91>!	8.6E10	0.	-0.5E3	
O2+B5CH2=HCHO+B1O 256) <DAGAUT91>!	1.0E14	0.	4.5E3	!(256,-
O2+R4CH3 (+M)=R8CH3OO (+M) 257) <BAULCH94>!	7.8E8	1.2	0.	!(257,-
LOW /5.6E25	-3.3	0./		
TROE /0.36	1.0	1.0E8/		
O2+R4CH3=R7CH3O+B1O 258) <BAULCH94>!	1.3E14	0.	31.3E3	!(258,-
O2+R4CH3=HCHO+R2OH 259) <DAGAUT91>!	3.0E30	-4.69	36.6E3	!(259,-
O2+CH4=R4CH3+R3OOH 260) <BAULCH94>!	4.0E13	0.	56.7E3	!(260,-
O2+R9C2HT=B2CO+R5CHO 261) <TIESEMANN97/TSANG86>!	3.8E13	-0.16	0.	!(261,-
O2+R9C2HT=R12CHCOV+B1O 262) <TIESEMANN97/TSANG86>!	9.0E12	-0.16	0.	!(262,-
O2+C2H2T=R9C2HT+R3OOH 263) <TSANG86>!	1.2E13	0.	74.5E3	!(263,-
O2+C2H2T=R5CHO+R5CHO 264) <BENSON95>!	7.0E7	1.8	30.6E3	!(264,-
O2+R10C2H3V=C2H2T+R3OOH 265) <MEBEL NIST>!	1.34E6	1.61	-0.4E3	!(265,-
O2+R10C2H3V=HCHO+R5CHO 266a) <MEBEL NIST>!	4.5E16	-1.39	1.0E3	!(266a,-
O2+R10C2H3V=B1O+R13CH2CHO 266b) <MEBEL NIST>!	3.3E11	-0.29	10.	!(266b,-
O2+C2H4Z=R10C2H3V+R3OOH 267) <TSANG86>!	4.2E13	0.	57.4E3	!(267,-
O2+R11C2H5=R17C2H5OO 268) <WAGNER90>!	2.2E10	0.77	-0.6E3	!(268,-

O2+R11C2H5=C2H4Z+R3OOH 269) <TSANG86>!	8.4E11	0.	3.9E3 ! (269,-
O2+R11C2H5=R15C2H5O+B1O 270) <BOZZELLI90NIST>!	1.2E13	-0.2	27.9E3 ! (270,-
O2+R11C2H5=CH3CHO+R2OH 271) <TSANG86>!	6.0E10	0.	6.9E3 ! (271,-
O2+C2H6=R11C2H5+R3OOH 272) <BAULCH94>!	6.0E13	0.	51.7E3 ! (272,-
O2+R2OH=R3OOH+B1O 273) <TSANG86>!	2.2E13	0.	52.5E3 ! (273,-
O2+B2CO=CO2+B1O 274) <TSANG86>!	2.5E12	0.	47.7E3 ! (274,-
O2+R5CHO=B2CO+R3OOH 275) <TIMONEN88>!	7.6E12	0.	0.41E3 ! (275,-
O2+HCHO=R5CHO+R3OOH 276) <TSANG86>!	2.0E13	0.	38.8E3 ! (276,-
O2+R7CH3O=HCHO+R3OOH 277) <BAULCH94>!	2.2E10	0.	1.7E3 ! (277,-
O2+R6CH2OH=HCHO+R3OOH 278) <TSANG87>!	1.2E12	0.	0. ! (278,-
O2+CH3OH=R6CH2OH+R3OOH 279) <TSANG87>!	2.0E13	0.	44.9E3 ! (279,-
O2+R12CHCOV=>B2CO+B2CO+R2OH <DAGAUT91>!	1.5E12	0.	2.5E3 ! (280)
O2+R14CH3CO=R18CH3COOO 282) <COX90>!	2.4E12	0.	0. ! (282,-
O2+R13CH2CHO=>HCHO+R2OH+B2CO <COX90>!	5.9E9	0.	-1.4E3 ! (283)
O2+R13CH2CHO=CH2COZ+R3OOH 284) <COX90>!	1.0E10	0.	-1.4E3 ! (284,-
O2+CH3CHO=R14CH3CO+R3OOH 285) <COX90>!	5.0E13	0.	36.4E3 ! (285,-
O2+CH3CHO=R13CH2CHO+R3OOH 285) <Ranzi94>!	1.0E13	0.5	46.0E3 ! (285',-
O2+C2H4OE#3=R3OOH+R13CH2CHO 286) <RANZI94>!	5.0E13	0.	48.0E3 ! (286,-
O2+R15C2H5O=CH3CHO+R3OOH 287) <BAULCH94>!	6.0E10	0.	1.7E3 ! (287,-
!REACTIONS DE R3OOH!			
R3OOH+R1H=H2+O2 288) <BAULCH94>!	4.3E13	0.	1.4E3 ! (288,-
R3OOH+R1H=2R2OH 289) <BAULCH94>!	1.7E14	0.	0.9E3 ! (289,-
R3OOH+R1H=H2O+B1O 290) <BAULCH94>!	3.0E13	0.	1.7E3 ! (290,-
R3OOH+B6CH2=HCHO+R2OH 291) <TSANG86>!	3.0E13	0.	0. ! (291,-
R3OOH+B5CH2=HCHO+R2OH 292) <TSANG86>!	1.8E13	0.	0. ! (292,-
R3OOH+R4CH3=R7CH3O+R2OH 293) <BAULCH94>!	1.8E13	0.	0. ! (293,-
!R3OOH+R4CH3=R7CH3O+R2OH 293) <DAGAUT>	4.0E13	0.	5.0E3 ! (293,-
R3OOH+CH4=R4CH3+H2O2 294) <BAULCH94>!	9.0E12	0.	24.6E3 ! (294,-
R3OOH+R9C2HT=R12CHCOV+R2OH 295) <TSANG86>!	1.8E13	0.	0. ! (295,-

R3OOH+C2H2T=CH2COZ+R2OH	6.0E9	0.	8.0E3	!(296,-
296)<TSANG86>!				
!incertitude au moins un facteur 10				
R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO	3.0E13	0.	0.	!(297)
<TSANG86>!				
R3OOH+C2H4Z=CH3CHO+R2OH	6.0E9	0.	7.9E3	!(298,-
298)<TSANG86>!				
R3OOH+C2H4Z=C2H4OE#3+R2OH	2.2E12	0.	17.2E3	!(299,-
299)<BAULCH94>!				
R3OOH+R11C2H5=>R4CH3+HCHO+R2OH	2.4E13	0.	0.	!(300)
<TSANG86>!				
R3OOH+R11C2H5=C2H4Z+H2O2	3.0E11	0.	0.	!(301,-
301)<TSANG86>!				
R3OOH+C2H6=R11C2H5+H2O2	1.3E13	0.	20.4E3	!(302,-
302)<BAULCH94>!				
R3OOH+R2OH=H2O+O2	2.9E13	0.	-0.5E3	!(303,-
303)<BAULCH94>!				
R3OOH+B2CO=CO2+R2OH	1.57E5	2.18	17.9E3	!(304,-
304)<TSANG86>; nouvelles donnees M. Cord !				
R3OOH+R5CHO=>R2OH+R1H+CO2	3.0E13	0.	0.	!(305)
<TSANG86>!				
R3OOH+HCHO=R5CHO+H2O2	3.0E12	0.	13.0E3	!(306,-
306)<BAULCH94>!				
R3OOH+R7CH3O=HCHO+H2O2	3.0E11	0.	0.	!(307,-
307)<TSANG86>!				
R3OOH+R6CH2OH=HCHO+H2O2	1.2E13	0.	0.	!(308,-
308)<TSANG87>!				
R3OOH+CH3OH=R6CH2OH+H2O2	9.6E10	0.	12.6E3	!(309,-
309)<TSANG87>!				
R3OOH+R14CH3CO=>R4CH3+CO2+R2OH	3.0E13	0.	0.	!(310)<TSANG86>!
!(310)<TSANG86>!				
R3OOH+CH3CHO=R14CH3CO+H2O2	1.0E12	0.	10.0E3	!(311,-
311)<CAVANAGH90>!				
R3OOH+C2H4OE#3=H2O2+R13CH2CHO	1.6E12	0.	15.0E3	!(312,-
312)<RANZI94>				
R3OOH+R3OOH=H2O2+O2	1.3E11	0.	-1.63E3	!(313,-
313)<BAULCH 94>!				
DUPLICATE				
R3OOH+R3OOH=H2O2+O2	4.2E14	0.	11.98E3	!(313,-
313)<BAULCH 94>!				
DUPLICATE				
!REACTIONS DE H2O2!				
R2OH+R2OH(+ M)=>H2O2 (+ M)	7.23E13	-0.37	0.00	
!(314)<BAULCH94>!				
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
N2/0.4/ HE/0.35/				
LOW /5.53E19 -0.76 0.00 /				
TROE /0.5 1 1.E8/				
H2O2(+M)=>R2OH+R2OH(+M)	3.00E14	0.00	48.5E3	!(-
314)<BAULCH94>!				
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
N2/0.4/ HE/0.35/				
LOW /3.0E17 0.0 45.5E3/				
TROE /0.5 1. 1.E8/				
H2O2+R1H=H2+R3OOH	1.7E12	0.	3.7E3	!(315,-
315)<BAULCH94>!				

H2O2+R1H=H2O+R2OH 316) <BAULCH94>!	1.0E13	0.	3.6E3 ! (316,-
H2O2+B6CH2=R7CH3O+R2OH 317) <TSANG86>!	3.0E13	0.	0. ! (317,-
H2O2+R10C2H3V=C2H4Z+R3OOH 318) <TSANG86>!	1.2E10	0.	-0.6E3 ! (318,-
H2O2+B1O=R2OH+R3OOH 319) <BAULCH94>!	6.6E11	0.	4.0E3 ! (319,-
H2O2+R2OH=H2O+R3OOH 320) <BAULCH94>!	7.8E12	0.	1.3E3 ! (320,-
!REACTIONS DE CO2!			
CO2+B5CH2=HCHO+B2CO 321) <TSANG86>!	2.3E10	0.	0. ! (321,-
!REACTIONS DE R8CH3OO!			
R8CH3OO=HCHO+R2OH 322) <RANZI94>!	1.5E13	0.	47.0E3 ! (322,-
R8CH3OO+R1H=R7CH3O+R2OH 323) <TSANG86>!	9.6E13	0.	0. ! (323,-
R8CH3OO+H2=CH3OOH+R1H 324) <TSANG86>!	3.0E13	0.	26.0E3 ! (324,-
R8CH3OO+B6CH2=HCHO+R7CH3O 325) <TSANG86>!	1.8E13	0.	0. ! (325,-
R8CH3OO+B5CH2=HCHO+R7CH3O 326) <TSANG86>!	1.8E13	0.	0. ! (326,-
R8CH3OO+R4CH3=R7CH3O+R7CH3O 327) <CAVANAGH90>!	5.0E12	0.	-1.4E3 ! (327,-
R8CH3OO+CH4=CH3OOH+R4CH3 328) <TSANG86>!	1.8E11	0.	18.5E3 ! (328,-
R8CH3OO+R9C2HT=R7CH3O+R12CHCOV 329) <TSANG86>!	2.4E13	0.	0. ! (329,-
R8CH3OO+C2H2T=CH3OOH+R9C2HT 330) <RANZI94>!	5.6E11	0.	24.5E3 ! (330,-
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 331) <TSANG86*>!	2.4E13	0.	0. ! (331,-
!* assuming that C2H3O decompose rapidly to R13CH2CHO!			
R8CH3OO+C2H4Z=R7CH3O+C2H4OE#3 332) <NIKISHA81/MOSHKINA80NIST>!	1.1E15	0.	20.0E3 ! (332,-
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V 333) <RANZI94>!	3.9E12	0.	24.5E3 ! (333,-
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O 334) <TSANG86>!	2.4E13	0.	0. ! (334,-
R8CH3OO+C2H6=CH3OOH+R11C2H5 335) <TSANG86>!	2.9E11	0.	14.9E3 ! (335,-
R8CH3OO+B1O=R7CH3O+O2 336) <TSANG86>!	3.6E13	0.	0. ! (336,-
R8CH3OO+R2OH=CH3OH+O2 337) <TSANG86>!	6.0E13	0.	0. ! (337,-
R8CH3OO+R2OH=R7CH3O+R3OOH 338) <RANZI94>!	3.0E12	0.	0. ! (338,-
R8CH3OO+B2CO=R7CH3O+CO2 339) <RANZI94>!	1.0E14	0.	24.0E3 ! (339,-
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2 <TSANG86>!	3.0E13	0.	0. ! (340)
R8CH3OO+HCHO=CH3OOH+R5CHO 341) <CAVANAGH90>!	1.0E12	0.	12.1E3 ! (341,-

R8CH3OO+R7CH3O=HCHO+CH3OOH	3.0E11	0.	0. ! (342,-
342) <TSANG86>!			
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO	1.2E13	0.	0.
! (343) <TSANG87>!			
R8CH3OO+CH3OH=CH3OOH+R6CH2OH	1.8E12	0.	13.7E3 ! (344,-
344) <TSANG87>!			
R8CH3OO+CH3OH=CH3OOH+R7CH3O	2.8E11	0.	18.8E3 ! (345,-
345) <RANZI94>!			
R8CH3OO+CH2COZ=CH3OOH+R12CHCOV	1.7E12	0.	27.0E3 ! (346,-
346) <RANZI94>!			
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O	2.4E13	0.	0. ! (347,-
347) <TSANG86>!			
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO	1.0E12	0.	12.1E3 ! (348,-
348) <CAVANAGH90>!			
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO	1.7E12	0.	19.2E3 ! (349,-
349) <RANZI94>!			
R8CH3OO+C2H4OE#3=CH3OOH+R13CH2CHO	2.2E12	0.	16.0E3 ! (350,-
350) <RANZI94>!			
R8CH3OO+R3OOH=CH3OOH+O2	2.5E11	0.	-1.6E3 ! (351,-
351) <BAULCH94>!			
R8CH3OO+R3OOH=>O2+HCHO+H2O	5.0E10	0.	0.
! (352) <RANZI94>!			
R8CH3OO+H2O2=CH3OOH+R3OOH	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 CH3OOH!			
CH3OOH=R7CH3O+R2OH	6.0E14	0.	42.3E3 ! (356,-
356) <BAULCH94>!			
CH3OOH+B1O=R8CH3OO+R2OH	2.0E13	0.	4.8E3 ! (357,-
357) <BAULCH94average>!			
CH3OOH+R2OH=H2O+R8CH3OO	1.8E12	0.	-0.37E3 ! (358,-
358) <BAULCH94average>!			
CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO	1.5E11	0.	6.5E3
! (359) <RANZI94>!			
!REACTIONS DE R17C2H5OO!			
R17C2H5OO=R16C2H4OOH	4.2E12	0.	36.9E3 ! (360,-
360) <HUGHES93>!			
R17C2H5OO+H2=C2H5OOH+R1H	7.9E12	0.	21.0E3 ! (361,-
361) <RANZI94>!			
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O	2.0E12	0.	-1.2E3 ! (362,-
362) <RANZI94>!			
R17C2H5OO+CH4=C2H5OOH+R4CH3	3.9E12	0.	24.0E3 ! (363,-
363) <RANZI94>!			
R17C2H5OO+C2H2T=C2H5OOH+R9C2HT	5.6E11	0.	24.4E3 ! (364,-
364) <RANZI94>!			
R17C2H5OO+C2H4Z=C2H5OOH+R10C2H3V	3.9E12	0.	24.4E3 ! (365,-
365) <RANZI94>!			
R17C2H5OO+C2H4Z=R15C2H5O+C2H4OE#3	2.3E16	0.	21.9E3 ! (366,-
366) <MOSHKINA80NIST>!			
R17C2H5OO+C2H6=C2H5OOH+R11C2H5	5.1E12	0.	19.5E3 ! (367,-
367) <RANZI94>!			
R17C2H5OO+H2O=C2H5OOH+R2OH	5.6E12	0.	30.6E3 ! (368,-
368) <RANZI94>!			



R17C2H500+B2CO=CO2+R15C2H5O 369) <RANZI94>!	1.0E14	0.	24.0E3 ! (369,-
R17C2H500+HCHO=C2H5OOH+R5CHO 370) <RANZI94>!	4.5E12	0.	14.4E3 ! (370,-
R17C2H500+CH3OH=C2H5OOH+R7CH3O 371) <RANZI94>!	2.8E11	0.	18.4E3 ! (371,-
R17C2H500+CH3OH=C2H5OOH+R6CH2OH 372) <RANZI94>!	2.8E12	0.	19.5E3 ! (372,-
R17C2H500+CH2COZ=C2H5OOH+R12CHCOV 373) <RANZI94>!	1.7E12	0.	24.4E3 ! (373,-
R17C2H500+CH3CHO=C2H5OOH+R14CH3CO 374) <RANZI94>!	3.9E12	0.	14.4E3 ! (374,-
R17C2H500+CH3CHO=C2H5OOH+R13CH2CHO 375) <RANZI94>!	1.7E12	0.	19.5E3 ! (375,-
R17C2H500+C2H4OE#3=C2H5OOH+R13CH2CHO 376) <RANZI94>!	2.2E12	0.	16.3E3 ! (376,-
R17C2H500+R3OOH=O2+C2H5OOH 377) <BAULCH89>!	3.9E11	0.	-1.3E3 ! (377,-
!Rate constant measured between 240 and 380K!			
R17C2H500+H2O2=C2H5OOH+R3OOH 378) <RANZI94>!	4.5E11	0.	10.8E3 ! (378,-
R17C2H500+R8CH3OO=>R15C2H5O+R7CH3O+O2 ! (379) <RANZI94>!	2.0E11	0.	0.
R17C2H500+CH3OOH=C2H5OOH+R8CH3OO 380) <RANZI94>!	1.1E12	0.	16.3E3 ! (380,-
R17C2H500+R17C2H500=2R15C2H5O+O2 381) <LIGHTFOOT92>!	4.1E10	0.	0.2E3 ! (381,-
R17C2H500+R17C2H500=C2H5OH+CH3CHO+O2 382) <LIGHTFOOT92>!	1.8E10	0.	0.2E3 ! (382,-
!REACTIONS DE R16C2H4OOH!			
R16C2H4OOH=C2H4OE#3+R2OH 383) <RANZI94>!	1.5E11	0.	20.0E3 ! (383,-
R16C2H4OOH=R6CH2OH+HCHO 384) <RANZI94>!	2.5E13	0.	27.5E3 ! (384,-
R16C2H4OOH=C2H4Z+R3OOH 385) <RANZI94>!	2.0E13	0.	23.5E3 ! (385,-
!REACTIONS DE C2H5OOH			
C2H5OOH=R15C2H5O+R2OH 386) <BAULCH94>!	4.0E15	0.	42.9E3 ! (386,-
C2H5OOH+R1H=>CH3CHO+R2OH+H2 ! (387) <RANZI94>!	3.2E13	0.	7.7E3
C2H5OOH+R4CH3=>CH3CHO+R2OH+CH4 ! (388) <RANZI94>!	5.7E11	0.	8.7E3
C2H5OOH+R9C2HT=>CH3CHO+R2OH+C2H2T ! (389) <RANZI94>!	6.0E11	0.	9.2E3
C2H5OOH+R10C2H3V=>CH3CHO+R2OH+C2H4Z ! (390) <RANZI94>!	1.0E12	0.	8.7E3
C2H5OOH+R11C2H5=>CH3CHO+R2OH+C2H6 ! (391) <RANZI94>!	3.4E11	0.	11.4E3
C2H5OOH+R2OH=>CH3CHO+R2OH+H2O ! (392) <RANZI94>!	5.9E12	0.	0.9E3
C2H5OOH+R5CHO=>CH3CHO+R2OH+HCHO ! (393) <RANZI94>!	1.8E12	0.	16.7E3
C2H5OOH+R7CH3O=>CH3CHO+R2OH+CH3OH ! (394) <RANZI94>!	6.3E11	0.	5.5E3

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C2H5OOH+R6CH2OH=>CH3CHO+R2OH+CH3OH  4.2E11      0.      13.6E3
!(395)<RANZI94>!
C2H5OOH+R14CH3CO=>2CH3CHO+R2OH      2.0E12      0.      18.5E3
!(396)<RANZI94>!
C2H5OOH+R13CH2CHO=>2CH3CHO+R2OH      3.4E11      0.      15.7E3
!(397)<RANZI94>!
C2H5OOH+R3OOH=>CH3CHO+R2OH+H2O2      8.0E11      0.      16.2E3
!(398)<RANZI94>!
C2H5OOH+R8CH3OO=>CH3CHO+R2OH+CH3OOH  1.1E12      0.      16.7E3
!(399)<RANZI94>!
C2H5OOH+R17C2H5OO=>CH3CHO+R2OH+C2H5OOH  1.1E12      0.      16.7E3
!(400)<RANZI94>!

!REACTIONS DE R18CH3COOO!
R18CH3COOO+C2H4OE#3=CH3COOOH+R13CH2CHO  1.0E12      0.      9.3E3
!(401,-402)<RANZI94>!
R18CH3COOO+R3OOH=CH3COOOH+O2          5.5E10      0.     -2.6E3
!(402,-402)<COX90>!
R18CH3COOO+C2H5OOH=CH3COOOH+R17C2H5OO  5.0E11      0.      9.2E3
!(403,-403)<RANZI94>!
R18CH3COOO+C2H5OOH=>CH3CHO+R2OH+CH3COOOH  5.0E11      0.      9.2E3
!(404)<RANZI94>!
R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2  1.7E12      0.     -1.0E3
!(405)<CAVANAGH90>!

!REACTIONS DE CH3COOOH!
CH3COOOH=>R4CH3+CO2+R2OH              1.0E16      0.     40.0E3
!(406)<CAVANAGH90>!

!REACTIONS DE R21CH3OCO = CH3-O-C(.)=O
R4CH3+CO2=R21CH3OCO                    4.76E7      1.54     3.47E4 !
<GLAUDE05>!
R7CH3O+B2CO=R21CH3OCO                   1.55E6      2.02     5.73E3 !
<GLAUDE05>!

! REACTIONS DE R22CO2H = O=C(.)-OH
R22CO2H(+M)=B2CO+R2OH(+M)              5.9E+12  0.53  33980 ! Larson
LOW / 2.20E23 -1.83  35260.0 /
R22CO2H(+M)=CO2+R1H(+M)                1.7E+12  0.31  32920 ! Larson
LOW / 2.9E26 -3.02  35070.0 /

! REACTION DE R23C2H3O2B
R23C2H3O2B=>CO2+R4CH3  1.70E9      1.0  38640

!*****

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

!REACTIONS PRODUISANT DES C2+ MOLECULAIRES
!REACTIONS DE R9C2HT!
!R9C2HT+R9C2HT=>C4H2                    1.8E13      0.      0.
!(24,-24)<TSANG86>!

!REACTIONS DE C2H2T!

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!C2H2T+B6CH2=>C3H4	1.7E14	0.	0.
! (27, -27) <BAULCH94>!			
!C2H2T+B5CH2=>C3H4	3.5E12	0.	0.
! (28, -28) <TSANG86>!			
!C2H2T+R4CH3=>C3H4+R1H	6.7E19	-2.08	31.6E3
! (29, -29) <DEAN87>!			
!C2H2T+R9C2HT=>C4H2+R1H	9.0E13	0.	0.
! (30, -30) <BAULCH94>!			
!C2H2T+C2H2T=>C4H4	5.5E12	0.	37.0E3
! (31, -31) <DURAN89>!			
!REACTIONS DE C2H3!			
!R10C2H3V+R4CH3=>C3H6Y	2.5E13	0.	0.
! (37, -37) <TSANG86>!			
!R10C2H3V+R9C2HT=>C4H4	1.8E13	0.	0.
! (38, -38) <TSANG86>!			
!R10C2H3V+C2H2T=>C4H4+R1H	2.0E12	0.	5.0E3
! (40, -40) <FAHR89>!			
!R10C2H3V+R10C2H3V=>C4H6YZ	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+R9C2HT=>C4H4+R1H	1.2E13	0.	0.
! (50, -50) <TSANG86>!			
!C2H4Z+R4CH3=>C3H6Y+R1H	6.6E11	0.	15.9E3
! <TSANG86>!			
!C2H4Z+R10C2H3V=>C4H6YZ+R1H	5.0E11	0.	7.3E3
! (51, -51) <TSANG86>!			
!REACTIONS DE C2H5!			
R11C2H5+R10C2H3V=>nC4H8Y	1.5E13	0.	0.
! (61, -61) <TSANG86>!			
R11C2H5+R11C2H5=>C4H10	1.1E13	0.	0.
! (65, -65) <BAULCH94>!			
!REACTIONS DE HCO!			
R5CHO+R10C2H3V=>C2H3CHOZ	1.8E13	0.	0.
! (138, -138) <TSANG86>!			
R5CHO+R11C2H5=>C2H5CHO	1.8E13	0.	0.
! (141, -141) <TSANG86>!			
!REACTIONS DE CH3O!			
!R7CH3O+R4CH3=CH3OCH3	1.2E13	0.	0.
! (159, -159) <TSANG86>!			
!R7CH3O+R7CH3O=>CH3OOCH3	1.8E12	0.	0.
! (172, -172) <TSANG86>!			
!REACTIONS DE CH2OH!			
R6CH2OH+R11C2H5=C3H7OH	1.2E13	0.	0.
! (189, -189) <TSANG87>!			
!REACTIONS DE CH3CO!			

R14CH3CO+R4CH3=>C2H6CO !(231,-231)<TSANG86>!	4.0E15	-0.8	0.
R14CH3CO+R11C2H5=>C3H8CO !(232,-232)<TSANG86>!	3.1E14	-0.5	0.
!R14CH3CO+R5CHO=>CH3COCHO !(237,-237)<TSANG86>!	1.8E13	0.	0.
!R14CH3CO+R6CH2OH=>CH3COCH2OH !(241,-241)<TSANG87>!	1.2E13	0.	0.
!R14CH3CO+R14CH3CO=>CH3COCOCH3 !(243,-243)<TSANG86>!	1.2E13	0.	12.3E3

!REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE

!C3H6Y+B1O=CH3CHCO+2R1H !<TSANG91>!	5.0E7	1.76	-1.22E3
!CH3CHCO+R2OH=B2CO+R10C2H3V+H2O !<MARINOV>!	4.0E6	2.0	0.0
!CH3CHCO+B1O=B2CO+R10C2H3V+R2OH !<MARINOV>!	7.2E12	0.0	2.0E3
!CH3CHCO+R1H=B2CO+R10C2H3V+H2 !<MARINOV>!	2.0E5	2.5	2.5E3
!CH3CHCO+R1H=R11C2H5+B2CO !<MARINOV>!	2.0E13	0.0	2.0E3
!CH3CHCO+B1O=R4CH3+R5CHO+B2CO !<MARINOV>!	3.0E7	2.0	0.0
!tC3H5+O2=CH3CHCO+R1H+B1O !<MARINOV>!	1.6E15	-0.78	3.1E3
!tC3H5+B1O=CH3CHCO+R1H !<MARINOV>!	1.0E14	0.0	0.0E3
!aC4H5+O2=CH3CHCO+R5CHO !<SLAGLE92>!	4.2E10	0.0	2.5E3
C2H3CHOZ+R2OH=B2CO+R10C2H3V+H2O !<MARINOV>!	1.0E13	0.0	0.0
C2H3CHOZ+B1O=B2CO+R10C2H3V+R2OH !<MARINOV>!	7.2E12	0.0	2.0E3
C2H3CHOZ+B1O=CH2COZ+R5CHO+R1H !<MARINOV>!	5.0E7	1.76	0.08E3
C2H3CHOZ+R1H=B2CO+R10C2H3V+H2 !<MARINOV>!	4.0E13	0.0	4.2E3
C2H3CHOZ+R1H=C2H4Z+R5CHO !<MARINOV>!	2.0E13	0.0	3.5E3
C2H3CHOZ+O2=B2CO+R10C2H3V+R3OOH !<MARINOV>!	3.0E13	0.0	36.0E3
!.C3H5Y+R3OOH=C2H3CHOZ+R1H+R2OH !<TSANG91>!	7.0E18	-2.0	0.0
!.C3H5Y+O2=C2H3CHOZ+R2OH !<BOZELLI93>!	1.8E13	-0.41	22.9E3
!.C3H5Y+B1O=C2H3CHOZ+R1H !<SLAGLE92>!	1.8E14	0.0	0.0

END