

! Automatically generated names by Genesys:
! Molecular formula
! +r if radical
! +_Olef if C=C double bond
! _number to distinguish between isomers

! InChI can be converted to molecular structure via
! <http://www.chemspider.com/StructureSearch.aspx>
! <http://www.chemicalize.org/>
! http://rmg.mit.edu/molecule_search
! or programs such as ChemDraw

ELEMENTS

AR HE C N O H
END

SPECIES

AR !! InChI=1S/Ar
C !! InChI=1S/C
C10H13r_Olef !! InChI=1S/C10H13/c1-5-9(3)7-8-10(4)6-2/h5-7H,1-4,8H2
HX15DE25V !! InChI=1S/C10H14/c1-5-9(3)7-8-10(4)6-2/h5-6H,1-4,7-8H2
C10H15r_Olef_3 !! InChI=1S/C10H15/c1-5-9(3)7-8-10(4)6-2/h5-6,9H,1-4,7-8H2
C10H15r_Olef !! InChI=1S/C10H15/c1-5-9(3)7-8-10(4)6-2/h5-6H,1,3-4,7-8H2,2H3
C10H15r_Olef_2 !! InChI=1S/C10H15/c1-5-9(3)7-8-10(4)6-2/h5-6H,1-3,7-8H2,4H3
C10H15r_Olef_1 !! InChI=1S/C10H15/c1-5-9(3)7-8-10(4)6-2/h5H,1-4,6-8H2
C2H !! InChI=1S/C2H/c1-2/h1H
C2H2 !! InChI=1S/C2H2/c1-2/h1-2H
H2CC !! InChI=1S/C2H2/c1-2/h1H2
HCCOH !! InChI=1S/C2H2O/c1-2-3/h1,3H
CH2CO !! InChI=1S/C2H2O/c1-2-3/h1H2
CHOCHO !! InChI=1S/C2H2O2/c3-1-2-4/h1-2H
C2H2O3 !! InChI=1S/C2H2O3/c3-1-2(4)5/h1H,(H,4,5)
C2H3 !! InChI=1S/C2H3/c1-2/h1H,2H2
C2H2OH !! InChI=1S/C2H3O/c1-2-3/h1-3H
CH3CO !! InChI=1S/C2H3O/c1-2-3/h1H3
CH2CHO !! InChI=1S/C2H3O/c1-2-3/h2H,1H2
C2H3O1-2 !! InChI=1S/C2H3O/c1-2-3-1/h1H,2H2
C2H3O2r !! InChI=1S/C2H3O2/c1-2(3)4/h1H2,(H,3,4)
CH3CO2 !! InChI=1S/C2H3O2/c1-2(3)4/h1H3
CH3OCO !! InChI=1S/C2H3O2/c1-4-2-3/h1H3
CH2OCHO !! InChI=1S/C2H3O2/c1-4-2-3/h2H,1H2
CH3CO3 !! InChI=1S/C2H3O3/c1-2(3)5-4/h1H3
O2CH2CHO !! InChI=1S/C2H3O3/c3-1-2-5-4/h1H,2H2
HO2CH2CO !! InChI=1S/C2H3O3/c3-1-2-5-4/h4H,2H2
OCH2OCHO !! InChI=1S/C2H3O3/c3-1-5-2-4/h1H,2H2
HOCH2OCO !! InChI=1S/C2H3O3/c3-1-5-2-4/h3H,1H2
C2H4 !! InChI=1S/C2H4/c1-2/h1-2H2
C2H3OH !! InChI=1S/C2H4O/c1-2-3/h2-3H,1H2
CH3CHO !! InChI=1S/C2H4O/c1-2-3/h2H,1H3
C2H4O1-2 !! InChI=1S/C2H4O/c1-2-3-1/h1-2H2
C2H3OOH !! InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2
CH3OCHO !! InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3
C2H4O2 !! InChI=1S/C2H4O2/c3-1-2-4/h1,4H,2H2

CH3CO3H !! InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3
 CHOCH2OOH !! InChI=1S/C2H4O3/c3-1-2-5-4/h1,4H,2H2
 HO2CH2OCHO !! InChI=1S/C2H4O4/c3-1-5-2-6-4/h1,4H,2H2
 C2H5 !! InChI=1S/C2H5/c1-2/h1H2,2H3
 SC2H4OH !! InChI=1S/C2H5O/c1-2-3/h2-3H,1H3
 C2H5O !! InChI=1S/C2H5O/c1-2-3/h2H2,1H3
 PC2H4OH !! InChI=1S/C2H5O/c1-2-3/h3H,1-2H2
 CH3OCH2 !! InChI=1S/C2H5O/c1-3-2/h1H2,2H3
 C2H5O2r !! InChI=1S/C2H5O2/c1-2-4-3/h2-3H,1H3
 C2H5O2 !! InChI=1S/C2H5O2/c1-2-4-3/h2H2,1H3
 C2H4O2H !! InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2
 CH3OCH2O !! InChI=1S/C2H5O2/c1-4-2-3/h2H2,1H3
 CH3OCH2O2 !! InChI=1S/C2H5O3/c1-4-2-5-3/h2H2,1H3
 CH2OCH2O2H !! InChI=1S/C2H5O3/c1-4-2-5-3/h3H,1-2H2
 C2H5O3r !! InChI=1S/C2H5O3/c3-1-2-5-4/h2-4H,1H2
 O2C2H4OH !! InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2
 O2CH2OCH2O2H !! InChI=1S/C2H5O5/c3-6-1-5-2-7-4/h3H,1-2H2
 C2H6 !! InChI=1S/C2H6/c1-2/h1-2H3
 C2H5OH !! InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3
 CH3OCH3 !! InChI=1S/C2H6O/c1-3-2/h1-2H3
 C2H5O2H !! InChI=1S/C2H6O2/c1-2-4-3/h3H,2H2,1H3
 CH3OCH2O2H !! InChI=1S/C2H6O3/c1-4-2-5-3/h3H,2H2,1H3
 HCCO !! InChI=1S/C2HO/c1-2-3/h1H
 O2CCHOOJ !! InChI=1S/C2HO4/c3-1(4)2(5)6/h(H,3,4) ?
 C3H2 !! InChI=1S/C3H2/c1-3-2/h1H2
 C3H2(S) !! InChI=1S/C3H2/c1-3-2/h1H2 - s
 H2CCC(S) !! InChI=1S/C3H2/c1-3-2/h1H2 - s#2
 C2HCHO !! InChI=1S/C3H2O/c1-2-3-4/h1,3H
 C3H3 !! InChI=1S/C3H3/c1-3-2/h1H,2H2
 CJ*CC*O !! InChI=1S/C3H3O/c1-2-3-4/h1-3H
 C3H3O !! InChI=1S/C3H3O/c1-2-3-4/h1H,3H2
 C2H3CO !! InChI=1S/C3H3O/c1-2-3-4/h2H,1H2
 HOC*CCJ*O !! InChI=1S/C3H3O2/c4-2-1-3-5/h1-2,4H
 CC3H4 !! InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2
 C3H4-A !! InChI=1S/C3H4/c1-3-2/h1-2H2
 C3H4-P !! InChI=1S/C3H4/c1-3-2/h1H,2H3
 C2H3CHO !! InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2
 CH3CHCO !! InChI=1S/C3H4O/c1-2-3-4/h2H,1H3
 C3H4O_olef !! InChI=1S/C3H4O/c1-2-3-4/h3-4H,1H2
 C3H3O2H !! InChI=1S/C3H4O2/c1-2-3-5-4/h1,4H,3H2
 CH3COCHO !! InChI=1S/C3H4O2/c1-3(5)2-4/h2H,1H3
 HOC*CC*O !! InChI=1S/C3H4O2/c4-2-1-3-5/h1-4H
 O(CH2)2CO !! InChI=1S/C3H4O2/c4-3-1-5-2-3/h1-2H2
 C3H5-S !! InChI=1S/C3H5/c1-3-2/h1,3H,2H3
 C3H5-T !! InChI=1S/C3H5/c1-3-2/h1H2,2H3
 C3H5-A !! InChI=1S/C3H5/c1-3-2/h3H,1-2H2
 CH3CHCHO !! InChI=1S/C3H5O/c1-2-3-4/h2-3H,1H3
 C3H5Or_olef_1 !! InChI=1S/C3H5O/c1-2-3-4/h2-4H,1H2
 C3H5O !! InChI=1S/C3H5O/c1-2-3-4/h2H,1,3H2
 C2H5CO !! InChI=1S/C3H5O/c1-2-3-4/h2H2,1H3
 PC3H4OH-2 !! InChI=1S/C3H5O/c1-2-3-4/h3-4H,1H3
 CH2CH2CHO !! InChI=1S/C3H5O/c1-2-3-4/h3H,1-2H2
 CH2CCH2OH !! InChI=1S/C3H5O/c1-2-3-4/h4H,1,3H2
 SC3H4OH !! InChI=1S/C3H5O/c1-3(2)4/h1,4H,2H3
 CH3COCH2 !! InChI=1S/C3H5O/c1-3(2)4/h1H2,2H3
 C3H5Or_olef !! InChI=1S/C3H5O/c1-3(2)4/h4H,1-2H2
 CCYCCO-T1 !! InChI=1S/C3H5O/c1-3-2-4-3/h2H2,1H3
 C2H3OCH2 !! InChI=1S/C3H5O/c1-3-4-2/h3H,1-2H2

C3H5O2r_Olef !! InChI=1S/C3H5O2/c1-2-3-5-4/h2-4H,1H2
CH3COCH2O !! InChI=1S/C3H5O2/c1-3(5)2-4/h2H2,1H3
CH3COCH2O2 !! InChI=1S/C3H5O3/c1-3(4)2-6-5/h2H2,1H3
CH2COCH2O2H!! InChI=1S/C3H5O3/c1-3(4)2-6-5/h5H,1-2H2
C3H6 !! InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3
C3H5OH !! InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2
SC3H5OH !! InChI=1S/C3H6O/c1-2-3-4/h2-4H,1H3
C2H5CHO !! InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3
C3H6O1-3 !! InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2
CH3COCH3 !! InChI=1S/C3H6O/c1-3(2)4/h1-2H3
IC3H5OH !! InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3
C3H6O1-2 !! InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3
CCY(COC)OH !! InChI=1S/C3H6O2/c1-2-3(4)5-2/h2-4H,1H3
AC3H5OOH !! InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2
IC3H5O !! InChI=1S/C3H6O2/c1-3(2)5-4/h4H,1H2,2H3
CHOCOCH3 !! InChI=1S/C3H6O2/c1-3(5)2-4/h2-3,5H,1H3
IC2H4OHCHO !! InChI=1S/C3H6O2/c1-3(5)2-4/h2-3,5H,1H3 - #2
CY(COC)COH !! InChI=1S/C3H6O2/c4-1-3-2-5-3/h3-4H,1-2H2
CY(CCOC)OH !! InChI=1S/C3H6O2/c4-3-1-2-5-3/h3-4H,1-2H2
C2H3COHOH !! InChI=1S/C3H6O3/c1-2-3(4)6-5/h2-5H,1H2
C3KET12 !! InChI=1S/C3H6O3/c1-3(2-4)6-5/h2-3,5H,1H3
CH2COHCH2OOH !! InChI=1S/C3H6O3/c1-3(4)2-6-5/h4-5H,1-2H2
CH3COCOHO !! InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3
C3KET21 !! InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3 - #2
C3KET13 !! InChI=1S/C3H6O3/c4-2-1-3-6-5/h2,5H,1,3H2
OHCOCOCH3!! InChI=1S/C3H6O4/c1-2(7-6)3(4)5/h2,6H,1H3,(H,4,5)
CHOCOCH2OOH !! InChI=1S/C3H6O4/c4-1-3(5)2-7-6/h1,3,5-6H,2H2
COHOHCY(COC) !! InChI=1S/C3H6O4/c4-3(7-5)2-1-6-2/h2-5H,1H2
OHCY(COCC)OOH !! InChI=1S/C3H6O4/c4-3-2(7-5)1-6-3/h2-5H,1H2
CH2CQCOHQ !! InChI=1S/C3H6O5/c1-2(7-5)3(4)8-6/h3-6H,1H2
CO(CH2OOH)2!! InChI=1S/C3H6O5/c4-3(1-7-5)2-8-6/h5-6H,1-2H2
NC3H7 !! InChI=1S/C3H7/c1-3-2/h1,3H2,2H3
IC3H7 !! InChI=1S/C3H7/c1-3-2/h3H,1-2H3
C3H6OH1-2 !! InChI=1S/C3H7O/c1-2-3-4/h2,4H,3H2,1H3
NC3H7O !! InChI=1S/C3H7O/c1-2-3-4/h2-3H2,1H3
C3H6OH2-1 !! InChI=1S/C3H7O/c1-3(2)4/h3-4H,1H2,2H3
IC3H7O !! InChI=1S/C3H7O/c1-3(2)4/h3H,1-2H3
TC3H6OH !! InChI=1S/C3H7O/c1-3(2)4/h4H,1-2H3
C3H6OOH1-2 !! InChI=1S/C3H7O2/c1-2-3-5-4/h2,4H,3H2,1H3
NC3H7O2 !! InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3
C3H6OOH1-3 !! InChI=1S/C3H7O2/c1-2-3-5-4/h4H,1-3H2
C3H6OOH2-1 !! InChI=1S/C3H7O2/c1-3(2)5-4/h3-4H,1H2,2H3
IC3H7O2 !! InChI=1S/C3H7O2/c1-3(2)5-4/h3H,1-2H3
C3H6OOH2-2 !! InChI=1S/C3H7O2/c1-3(2)5-4/h4H,1-2H3
TQC3H5OHI !! InChI=1S/C3H7O3/c1-3(2-4)6-5/h2-5H,1H3
TQC3H6OI !! InChI=1S/C3H7O3/c1-3(2-4)6-5/h3,5H,2H2,1H3
TQJC3H6OH !! InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-4H,2H2,1H3
QC3H5OHP !! InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-5H,1-2H2
IQJC3H6OH !! InChI=1S/C3H7O3/c1-3(4)2-6-5/h2-5H,1H3
IQC3H6OT !! InChI=1S/C3H7O3/c1-3(4)2-6-5/h3,5H,2H2,1H3
IQC3H5OHPJ !! InChI=1S/C3H7O3/c1-3(4)2-6-5/h3-5H,1-2H2
HOC3H6O2 !! InChI=1S/C3H7O3/c4-2-1-3-6-5/h4H,1-3H2
C3H6OOH2-1O2 !! InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3,5H,2H2,1H3
C3H6OOH1-2O2 !! InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-4H,2H2,1H3
C3H51-2,3OOH !! InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-5H,1-2H2
C3H52-1,3OOH !! InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h1,4-5H,2-3H2
C3H6OOH1-3O2 !! InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h4H,1-3H2
TQC3H5OHTO2!! InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2,4-6H,1H3

TQC3H5OHIO2 !! InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-5H,1H3
TQC3H5OHIQ-P !! InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-6H,1H2
TQC3H5OHIQ-I !! InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h3-6H,1H3
IQC3H5OHQ-SJ !! InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h1,3-6H,2H2
IQC3H5OTQ-I !! InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h3,5-6H,1-2H2
IQC3H5OHPJO2 !! InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h3-5H,1-2H2
C3H8 !! InChI=1S/C3H8/c1-3-2/h3H2,1-2H3
NC3H7O2H !! InChI=1S/C3H8O2/c1-2-3-5-4/h4H,2-3H2,1H3
IC3H7O2H !! InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3
C4H10 !! InChI=1S/C4H10/c1-3-4-2/h3-4H2,1-2H3
IC4H10 !! InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3
PC4H9O2H !! InChI=1S/C4H10O2/c1-2-3-4-6-5/h5H,2-4H2,1H3
SC4H9O2H !! InChI=1S/C4H10O2/c1-3-4(2)6-5/h4-5H,3H2,1-2H3
IC4H9O2H !! InChI=1S/C4H10O2/c1-4(2)3-6-5/h4-5H,3H2,1-2H3
TC4H9O2H !! InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3
C4H2 !! InChI=1S/C4H2/c1-3-4-2/h1-2H
C3H2C !! InChI=1S/C4H2/c1-3-4-2/h1H2
H2C4O !! InChI=1S/C4H2O/c1-2-3-4-5/h1,3H
C4H3-N !! InChI=1S/C4H3/c1-3-4-2/h1-3H
C4H3-I !! InChI=1S/C4H3/c1-3-4-2/h1H,2H2
C4H4 !! InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2
C4H4O_olef !! InChI=1S/C4H4O/c1-2-3-4-5/h3-4H,1H2
C4H4O !! InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H
C4H5-N !! InChI=1S/C4H5/c1-3-4-2/h1,3-4H,2H2
C4H5-2 !! InChI=1S/C4H5/c1-3-4-2/h1H2,2H3
C4H5-I !! InChI=1S/C4H5/c1-3-4-2/h3H,1-2H2
CH3CHCHCO !! InChI=1S/C4H5O/c1-2-3-4-5/h2-3H,1H3
SC3H5CO !! InChI=1S/C4H5O/c1-2-3-4-5/h2-3H,1H3 - #2
C*CCJC*O !! InChI=1S/C4H5O/c1-2-3-4-5/h2-4H,1H2
CH2CHCHCHO !! InChI=1S/C4H5O/c1-2-3-4-5/h2-4H,1H2 - #2
C4H5Or_olef_1 !! InChI=1S/C4H5O/c1-2-3-4-5/h3-4H,1H3
C*[C]CC*O !! InChI=1S/C4H5O/c1-2-3-4-5/h4H,1,3H2
C4H5Or_olef !! InChI=1S/C4H5O/c1-4(2)3-5/h1,3H,2H3
IC3H5C̄O !! InChI=1S/C4H5O/c1-4(2)3-5/h1H2,2H3
IC3H4CHO-A !! InChI=1S/C4H5O/c1-4(2)3-5/h3H,1-2H2
C4H5O2r_olef !! InChI=1S/C4H5O2/c1-2-3-4(5)6/h3H,1H3,(H,5,6)
OC4H5O !! InChI=1S/C4H5O2/c5-3-1-2-4-6/h1,3-4H,2H2
C4H6-2 !! InChI=1S/C4H6/c1-3-4-2/h1-2H3
C4H6 !! InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2
C4H612 !! InChI=1S/C4H6/c1-3-4-2/h4H,1H2,2H3
C4H6O_olef_6 !! InChI=1S/C4H6O/c1-2-3-4-5/h2,4-5H,1H3
C*CCC*O !! InChI=1S/C4H6O/c1-2-3-4-5/h2,4H,1,3H2
CH3CHCHCHO !! InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3
SC3H5CHO !! InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3 - #2
C4H6O_olef_4 !! InChI=1S/C4H6O/c1-2-3-4-5/h2-5H,1H2
C4H6O_olef !! InChI=1S/C4H6O/c1-2-3-4-5/h3,5H,1,4H2
C2H5CHCO !! InChI=1S/C4H6O/c1-2-3-4-5/h3H,2H2,1H3
C2H3CHOCH2 !! InChI=1S/C4H6O/c1-2-4-3-5-4/h2,4H,1,3H2
C4H6O23 !! InChI=1S/C4H6O/c1-2-4-5-3-1/h1,3H,2,4H2
C4H6O25 !! InChI=1S/C4H6O/c1-2-4-5-3-1/h1-2H,3-4H2
C4H6O_olef_5 !! InChI=1S/C4H6O/c1-3-4(2)5/h3,5H,1-2H2
C2H3COCH3 !! InChI=1S/C4H6O/c1-3-4(2)5/h3H,1H2,2H3
C4H6O_olef_7 !! InChI=1S/C4H6O/c1-3-4(2)5/h5H,1H2,2H3
IC3H6CO !! InChI=1S/C4H6O/c1-4(2)3-5/h1-2H3
IC3H5CHO !! InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3
C*CYCCOC !! InChI=1S/C4H6O/c1-4-2-5-3-4/h1-3H2
C4H6O2_olef !! InChI=1S/C4H6O2/c1-4(6)2-3-5/h2-3,5H,1H3
C4H6O2_olef_1 !! InChI=1S/C4H6O2/c1-4(6)2-3-5/h2-3,6H,1H3

C4H6O2 !! InChI=1S/C4H6O2/c1-4(6)2-3-5/h3H,2H2,1H3
OC4H6O !! InChI=1S/C4H6O2/c5-3-1-2-4-6/h3-4H,1-2H2
C4H6O3_1 !! InChI=1S/C4H6O3/c1-3(5)2-4(6)7/h2H2,1H3,(H,6,7)
C4H6O3_2 !! InChI=1S/C4H6O3/c1-3(6)4(7)2-5/h5H,2H2,1H3
C4H6O3 !! InChI=1S/C4H6O3/c5-2-1-4(7)3-6/h3,5H,1-2H2
C4H71-1 !! InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3
C4H71-2 !! InChI=1S/C4H7/c1-3-4-2/h1,4H2,2H3
C4H71-3 !! InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3
C4H71-4 !! InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2
C4H72-2 !! InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3
IC4H7 !! InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3
IC4H7-I1 !! InChI=1S/C4H7/c1-4(2)3/h1H,2-3H3
C3H6CHO-2 !! InChI=1S/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3
NC3H7CO !! InChI=1S/C4H7O/c1-2-3-4-5/h2-3H2,1H3
CCJ*CCOH !! InChI=1S/C4H7O/c1-2-3-4-5/h3,5H,4H2,1H3
C3H6CHO-3 !! InChI=1S/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3
C3H6CHO-1 !! InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2
C4H7Or_olef !! InChI=1S/C4H7O/c1-2-3-4-5/h5H,1,3-4H2
CH2CH2COCH3 !! InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3
C2H5COCH2 !! InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3
C*CCJ(C)OH !! InChI=1S/C4H7O/c1-3-4(2)5/h3,5H,1H2,2H3
C4H7O !! InChI=1S/C4H7O/c1-3-4(2)5/h3-4H,1H2,2H3
CH3CHCOCH3 !! InChI=1S/C4H7O/c1-3-4(2)5/h3H,1-2H3
IC4H7O !! InChI=1S/C4H7O/c1-4(2)3-5/h1,3H2,2H3
SC4H7OH-IP !! InChI=1S/C4H7O/c1-4(2)3-5/h3,5H,1H2,2H3
IC3H6CHO !! InChI=1S/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3
TC3H6CHO !! InChI=1S/C4H7O/c1-4(2)3-5/h3H,1-2H3
IC3H7CO !! InChI=1S/C4H7O/c1-4(2)3-5/h4H,1-2H3
IC4H6OH !! InChI=1S/C4H7O/c1-4(2)3-5/h5H,1-3H2
IC3H5OCH2 !! InChI=1S/C4H7O/c1-4(2)5-3/h1,3H2,2H3
C4H7O2r_3 !! InChI=1S/C4H7O2/c1-2-3-4(5)6/h2H,3H2,1H3,(H,5,6)
C4H7O2r_olef_2 !! InChI=1S/C4H7O2/c1-2-3-4-6-5/h2,4-5H,1,3H2
C4H7O2r_olef_1 !! InChI=1S/C4H7O2/c1-2-3-4-6-5/h2-5H,1H3
C4H7O2r_4 !! InChI=1S/C4H7O2/c1-2-4(6)3-5/h2,5H,3H2,1H3
CJC(OH)C(*O)C !! InChI=1S/C4H7O2/c1-3(5)4(2)6/h3,5H,1H2,2H3
C4H7O2r_6 !! InChI=1S/C4H7O2/c1-3(5)4(2)6/h3H,1-2H3
C4H7O2r_olef_3 !! InChI=1S/C4H7O2/c1-3-4(2)6-5/h3,5H,1H2,2H3
CCY(C2O)CO !! InChI=1S/C4H7O2/c1-3-4(2-5)6-3/h3-4H,2H2,1H3
C2CYCOOC-I1 !! InChI=1S/C4H7O2/c1-4(2)3-5-6-4/h1,3H2,2H3
IC4H7O2 !! InChI=1S/C4H7O2/c1-4(2)3-6-5/h1,3H2,2H3
C4H7O2r_olef !! InChI=1S/C4H7O2/c1-4(2)3-6-5/h3,5H,1H2,2H3
IC4H6OOH-I !! InChI=1S/C4H7O2/c1-4(2)3-6-5/h5H,1-3H2
TC3H6OCHO !! InChI=1S/C4H7O2/c1-4(2)6-3-5/h3H,1-2H3
IC3H5OCH2 !! InChI=1S/C4H7O2/c1-4(2)6-5-3/h1,3H2,2H3
C4H7O2r !! InChI=1S/C4H7O2/c1-4(2,6)3-5/h3H,1-2H3
CHOIC3H6O !! InChI=1S/C4H7O2/c1-4(2-5)3-6/h2,4H,3H2,1H3
CCYCCOOC-I2 !! InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2,4H,3H2,1H3
CCYCCOOC-T1 !! InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2-3H2,1H3
CH2CHOOHCOCH3 !! InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4,6H,2H2,1H3
CH3CHOOHCOCH3 !! InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3
C4H7O3r_1 !! InChI=1S/C4H7O3/c1-3(6)4(7)2-5/h4-5H,2H2,1H3
TC3H6O2CHO !! InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3H,1-2H3
TC3H6O2HCO !! InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h6H,1-2H3
IC3H5O2HCHO !! InChI=1S/C4H7O3/c1-4(2-5)3-7-6/h2,4,6H,1,3H2
C4H8-2 !! InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3
C4H8-1 !! InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3
IC4H8 !! InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3
CCYCCC !! InChI=1S/C4H8/c1-4-2-3-4/h4H,2-3H2,1H3

C*CCCOH !! InChI=1S/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2
C4H8O_olef_1 !! InChI=1S/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3
NC3H7CHO !! InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3
C4H8O1-2 !! InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3
C4H8O1-4 !! InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2
CC4H8O !! InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2 - #2
C2H5COCH3 !! InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3
C4H8O2-3 !! InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3
SC4H7OH-I !! InChI=1S/C4H8O/c1-4(2)3-5/h3,5H,1-2H3
IC3H7CHO !! InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3
IC4H7OH !! InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3
IC4H8O !! InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3
C4H8O1-3 !! InChI=1S/C4H8O/c1-4-2-5-3-4/h4H,2-3H2,1H3
AC4H7OOH !! InChI=1S/C4H8O2/c1-3-4-6-5-2/h3H,1,4H2,2H3
C2CY(COC)OH !! InChI=1S/C4H8O2/c1-4(2)3(5)6-4/h3,5H,1-2H3
IC4H7OOH !! InChI=1S/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3
IC3H6OHCHO !! InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3
TC3H6OHCHO !! InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3 - #2
CCY(CCO)COH !! InChI=1S/C4H8O2/c1-4(2-5)3-6-4/h5H,2-3H2,1H3
CCY(CCOC)OH !! InChI=1S/C4H8O2/c1-4(5)2-3-6-4/h5H,2-3H2,1H3
C4H8O2_olef_1 !! InChI=1S/C4H8O2/c1-4(6)2-3-5/h2,5-6H,3H2,1H3
NC4KET12 !! InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h3-4,6H,2H2,1H3
NC4KET21 !! InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h6H,2-3H2,1H3
IC3H5COHQ !! InChI=1S/C4H8O3/c1-3(2)4(5)7-6/h4-6H,1H2,2H3
NC4KET23 !! InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4,6H,1-2H3
IC4KETIT !! InChI=1S/C4H8O3/c1-4(2,3-5)7-6/h3,6H,1-2H3
IC4KETII !! InChI=1S/C4H8O3/c1-4(2-5)3-7-6/h2,4,6H,3H2,1H3
NC4KET24 !! InChI=1S/C4H8O3/c1-4(5)2-3-7-6/h6H,2-3H2,1H3
NC4KET13 !! InChI=1S/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3
NC4KET14 !! InChI=1S/C4H8O3/c5-3-1-2-4-7-6/h3,6H,1-2,4H2
C4H8O4 !! InChI=1S/C4H8O4/c1-3(6)4(2-5)8-7/h4-5,7H,2H2,1H3
HOCOCQ(CH3)2 !! InChI=1S/C4H8O4/c1-4(2,8-7)3(5)6/h7H,1-2H3,(H,5,6)
CH2C(CH2OOH)2 !! InChI=1S/C4H8O4/c1-4(2-7-5)3-8-6/h5-6H,1-3H2
CHOC(CH3)OHCH2Q !! InChI=1S/C4H8O4/c1-4(6,2-5)3-8-7/h2,6-7H,3H2,1H3
QCYC(CCOC)OH !! InChI=1S/C4H8O4/c1-4(8-6)2-7-3(4)5/h3,5-6H,2H2,1H3
COHQCYC(COC) !! InChI=1S/C4H8O4/c5-4(8-6)1-3-2-7-3/h3-6H,1-2H2
PC4H9 !! InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3
SC4H9 !! InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3
TC4H9 !! InChI=1S/C4H9/c1-4(2)3/h1-3H3
IC4H9 !! InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3
PC4H9O !! InChI=1S/C4H9O/c1-2-3-4-5/h2-4H2,1H3
SC4H8OH !! InChI=1S/C4H9O/c1-3-4(2)5/h3-5H,1-2H3
PC4H8OH !! InChI=1S/C4H9O/c1-3-4(2)5/h4-5H,2-3H2,1H3
SC4H9O !! InChI=1S/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3
IC4H9O !! InChI=1S/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3
IC4H8OH-IT !! InChI=1S/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3
IC4H8OH !! InChI=1S/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3 -#2
TC4H9O !! InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3
IC4H8OH-TI !! InChI=1S/C4H9O/c1-4(2,3)5/h5H,1H2,2-3H3
C4H8OOH1-3 !! InChI=1S/C4H9O2/c1-2-3-4-6-5/h2,5H,3-4H2,1H3
PC4H9O2 !! InChI=1S/C4H9O2/c1-2-3-4-6-5/h2-4H2,1H3
C4H8OOH1-2 !! InChI=1S/C4H9O2/c1-2-3-4-6-5/h3,5H,2,4H2,1H3
C4H8OOH1-1 !! InChI=1S/C4H9O2/c1-2-3-4-6-5/h4-5H,2-3H2,1H3
C4H8OOH1-4 !! InChI=1S/C4H9O2/c1-2-3-4-6-5/h5H,1-4H2
C4H8OOH2-3 !! InChI=1S/C4H9O2/c1-3-4(2)6-5/h3-5H,1-2H3
C4H8OOH2-4 !! InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,1,3H2,2H3
C4H8OOH2-1 !! InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,2-3H2,1H3
SC4H9O2 !! InChI=1S/C4H9O2/c1-3-4(2)6-5/h4H,3H2,1-2H3

C4H8OOH2-2 !! InChI=1S/C4H9O2/c1-3-4(2)6-5/h5H,3H2,1-2H3
C4H9O2r !! InChI=1S/C4H9O2/c1-4(2)3-6-5/h3-5H,1-2H3
IC4H8O2H-I !! InChI=1S/C4H9O2/c1-4(2)3-6-5/h4-5H,1,3H2,2H3
IC4H9O2 !! InChI=1S/C4H9O2/c1-4(2)3-6-5/h4H,3H2,1-2H3
IC4H8O2H-T !! InChI=1S/C4H9O2/c1-4(2)3-6-5/h5H,3H2,1-2H3
TC4H9O2 !! InChI=1S/C4H9O2/c1-4(2,3)6-5/h1-3H3
TC4H8O2H-I !! InChI=1S/C4H9O2/c1-4(2,3)6-5/h5H,1H2,2-3H3
C4H8OH-1O2 !! InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4-5H,2-3H2,1H3
C4H8OH-2O2 !! InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-5H,1-2H3
TQC4H7OHI !! InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h3,5-6H,1-2H3
QC4H7OHP !! InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5-6H,1,3H2,2H3
TQJC4H8OH !! InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5H,3H2,1-2H3
TQC4H8OI !! InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h6H,3H2,1-2H3
C4H9O3r !! InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h3,5-6H,1-2H3
IQC4H7OHT !! InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5-6H,1,3H2,2H3
IQJC4H8OH !! InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5H,3H2,1-2H3
IQC4H8OT !! InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h6H,3H2,1-2H3
C4H8OOH2-1O2 !! InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4,6H,2-3H2,1H3
C4H8OOH1-2O2 !! InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-5H,2-3H2,1H3
C4H8OOH2-3O2 !! InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-5H,1-2H3
C4H9O4r !! InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h3,5-6H,1-2H3
TIC4H7Q2-I !! InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5-6H,1,3H2,2H3
IC4H8OOH-TO2 !! InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5H,3H2,1-2H3
TC4H8OOH-IO2 !! InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h6H,3H2,1-2H3
IIC4H7Q2-I !! InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h2,4-6H,3H2,1H3
IC4H8OOH-IO2 !! InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-5H,2-3H2,1H3
IIC4H7Q2-T !! InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h5-6H,2-3H2,1H3
C4H8OOH2-4O2 !! InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4,6H,2-3H2,1H3
C4H8OOH1-3O2 !! InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-5H,2-3H2,1H3
C4H8OOH1-4O2 !! InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h5H,1-4H2
TQC4H7OHIO2 !! InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5,7H,1-2H3
TQC4H7OHIOQ-P !! InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5-7H,1H2,2H3
TQC4H7OHIOQ-I !! InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,6-7H,1-2H3
TQC4H7OHTO2 !! InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h5-7H,1-2H3
IQC4H7OHTO2 !! InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-6H,2-3H2,1H3
IQC4H7OHTQ-P !! InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-7H,1-3H2
IQC4H8OTQ-I !! InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h6-7H,2-3H2,1H3
C5H10_olef_1 !! InChI=1S/C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3
C*CCCC !! InChI=1S/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3
AC5H10 !! InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3
CC(C)C*C !! InChI=1S/C5H10/c1-4-5(2)3/h4-5H,1H2,2-3H3
CC(C)*CC !! InChI=1S/C5H10/c1-4-5(2)3/h4H,1-3H3
C5H10O_olef_2 !! InChI=1S/C5H10O/c1-4-5(2,3)6/h4,6H,1H2,2-3H3
Prenol !! InChI=1S/C5H10O/c1-5(2)3-4-6/h3,6H,4H2,1-2H3
C5H10O_olef !! InChI=1S/C5H10O/c1-5(2)3-4-6/h3-6H,1-2H3
CC(C)CC*O !! InChI=1S/C5H10O/c1-5(2)3-4-6/h4-5H,3H2,1-2H3
Isoprenol !! InChI=1S/C5H10O/c1-5(2)3-4-6/h6H,1,3-4H2,2H3
C5H10O2_olef_3m !! InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h3-4,6H,2,5H2,1H3
C5H10O2_18 !! InChI=1S/C5H10O2/c1-3(2)4-5(6)7-4/h3-6H,1-2H3
C5H10O2_olef_4m4 !! InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3-6H,1-2H3
C5H10O2_olef_14 !! InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,6H,4H2,1-2H3
C5H10O2_olef_10 !! InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h6H,2-4H2,1H3
C5H10O2_olef_1m !! InChI=1S/C5H10O2/c1-3-5(4-2)7-6/h3,5-6H,1,4H2,2H3
C5H10O2_olef_12 !! InChI=1S/C5H10O2/c1-4(2)5(3)7-6/h5-6H,1H2,2-3H3
CC(C)(OH)CCHO !! InChI=1S/C5H10O2/c1-4(2)5(7)3-6/h4,6H,3H2,1-2H3
C5H10O2_olef_2 !! InChI=1S/C5H10O2/c1-4(2)5(7)3-6/h5-7H,1,3H2,2H3
C5H10O2_olef_3 !! InChI=1S/C5H10O2/c1-4(2)5(7)3-6/h6-7H,3H2,1-2H3
C5H10O2_4 !! InChI=1S/C5H10O2/c1-4-2-5(6)7-3-4/h4-6H,2-3H2,1H3

C5H10O2_7 !! InChI=1S/C5H10O2/c1-4-3-7-5(4)2-6/h4-6H,2-3H2,1H3
C5H10O2_Olef_8 !! InChI=1S/C5H10O2/c1-4-5(2,3)7-6/h4,6H,1H2,2-3H3
C5H10O2_21 !! InChI=1S/C5H10O2/c1-4-5(2,6)3-7-4/h4,6H,3H2,1-2H3
C5H10O2_1 !! InChI=1S/C5H10O2/c1-5(2)3-4(6)7-5/h4,6H,3H2,1-2H3
C5H10O2_Olef_9 !! InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h3,6H,4H2,1-2H3
C5H10O2_2 !! InChI=1S/C5H10O2/c1-5(2)4(3-6)7-5/h4,6H,3H2,1-2H3
IC4H7OOC3 !! InChI=1S/C5H10O2/c1-5(2)4-7-6-3/h1,4H2,2-3H
C5H10O2_25 !! InChI=1S/C5H10O2/c1-5(2,6)4-3-7-4/h4,6H,3H2,1-2H3
C5H10O2_Olef !! InChI=1S/C5H10O2/c1-5(2,7)3-4-6/h3-4,6-7H,1-2H3
C5H10O2_13 !! InChI=1S/C5H10O2/c1-5(2-3-6)4-7-5/h6H,2-4H2,1H3
C5H10O2_23 !! InChI=1S/C5H10O2/c1-5(6)2-3-7-4-5/h6H,2-4H2,1H3
C5H10O2_8 !! InChI=1S/C5H10O2/c6-2-1-5-3-7-4-5/h5-6H,1-4H2
C5H10O3_Olef_6 !! InChI=1S/C5H10O3/c1-4(2)3-5(6)8-7/h3,5-7H,1-2H3
C5H10O3_3 !! InChI=1S/C5H10O3/c1-4(2)5(3-6)8-7/h3-5,7H,1-2H3
C5H10O3_Olef_2 !! InChI=1S/C5H10O3/c1-4(2)5(3-6)8-7/h5-7H,1,3H2,2H3
C5H10O3_13 !! InChI=1S/C5H10O3/c1-5(2)3(6)4(7)8-5/h3-4,6-7H,1-2H3
C5H10O3_12 !! InChI=1S/C5H10O3/c1-5(2,7)3-4(6)8-3/h3-4,6-7H,1-2H3
C5H10O3_Olef_1 !! InChI=1S/C5H10O3/c1-5(2,8-7)3-4-6/h3-4,6-7H,1-2H3
C5H10O3_2 !! InChI=1S/C5H10O3/c1-5(2,8-7)3-4-6/h4,7H,3H2,1-2H3
C5H10O3_Olef_5 !! InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h2,6-7H,3-4H2,1H3
C5H10O3 !! InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h3,5,7H,2,4H2,1H3
C*(C(COOH)CCOH) !! InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h6-7H,1-4H2
C5H10O3_16 !! InChI=1S/C5H10O3/c1-5(3-8-5)4(7)2-6/h4,6-7H,2-3H2,1H3
C5H10O3_6 !! InChI=1S/C5H10O3/c1-5(7)3-8-4(5)2-6/h4,6-7H,2-3H2,1H3
C5H10O4_12 !! InChI=1S/C5H10O4/c1-3(2)4(6)5(7)9-8/h3,5,7-8H,1-2H3
C5H10O4_10 !! InChI=1S/C5H10O4/c1-3(2)4(9-8)5(6)7/h3-4,8H,1-2H3,(H,6,7)
C5H10O4 !! InChI=1S/C5H10O4/c1-4(3-6)2-5(7)9-8/h3-5,7-8H,2H2,1H3
C5H10O4_7 !! InChI=1S/C5H10O4/c1-4(3-9-8)2-5(6)7/h4,8H,2-3H2,1H3,(H,6,7)
C5H10O4_14 !! InChI=1S/C5H10O4/c1-4(3-9-8)5(7)2-6/h4,6,8H,2-3H2,1H3
C5H10O4_8 !! InChI=1S/C5H10O4/c1-5(2,9-8)3-4(6)7/h8H,3H2,1-2H3,(H,6,7)
C5H10O4_15 !! InChI=1S/C5H10O4/c1-5(2,9-8)4(7)3-6/h6,8H,3H2,1-2H3
C5H10O4_5 !! InChI=1S/C5H10O4/c1-5(4-7,9-8)2-3-6/h4,6,8H,2-3H2,1H3
CJCCCC !! InChI=1S/C5H11/c1-3-5-4-2/h1,3-5H2,2H3
CCJCCC !! InChI=1S/C5H11/c1-3-5-4-2/h3H,4-5H2,1-2H3
CCCJCC !! InChI=1S/C5H11/c1-3-5-4-2/h5H,3-4H2,1-2H3
C5H11r_3 !! InChI=1S/C5H11/c1-4-5(2)3/h4-5H,1-3H3
C5H11r !! InChI=1S/C5H11/c1-4-5(2)3/h4H2,1-3H3
C5H11r_4 !! InChI=1S/C5H11/c1-4-5(2)3/h5H,1,4H2,2-3H3
C5H11r_1 !! InChI=1S/C5H11/c1-4-5(2)3/h5H,2,4H2,1,3H3
CC(C)CJCOH !! InChI=1S/C5H11O/c1-5(2)3-4-6/h3,5-6H,4H2,1-2H3
CC(C)CCJOH !! InChI=1S/C5H11O/c1-5(2)3-4-6/h4-6H,3H2,1-2H3
C5H11Or_1 !! InChI=1S/C5H11O/c1-5(2)3-4-6/h5-6H,1,3-4H2,2H3
CCJ(C)CCOH !! InChI=1S/C5H11O/c1-5(2)3-4-6/h6H,3-4H2,1-2H3
C5H11O2r !! InChI=1S/C5H11O2/c1-4(2)5(7)3-6/h5-7H,3H2,1-2H3
C5H11O2r_2 !! InChI=1S/C5H11O2/c1-5(2,7)3-4-6/h3,6-7H,4H2,1-2H3
C5H11O3r_25 !! InChI=1S/C5H11O3/c1-4(2)3-5(6)8-7/h3-7H,1-2H3
C5H11O3r_26 !! InChI=1S/C5H11O3/c1-4(2)3-5(6)8-7/h4-6H,3H2,1-2H3
C5H11O3r_30 !! InChI=1S/C5H11O3/c1-4(2)3-5(6)8-7/h4-7H,1,3H2,2H3
C5H11O3r_28 !! InChI=1S/C5H11O3/c1-4(2)3-5(6)8-7/h5-7H,3H2,1-2H3
C5H11O3r_23 !! InChI=1S/C5H11O3/c1-4(2)5(3-6)8-7/h3-7H,1-2H3
C5H11O3r_19 !! InChI=1S/C5H11O3/c1-4(2)5(3-6)8-7/h4-5,7H,3H2,1-2H3
C5H11O3r_16 !! InChI=1S/C5H11O3/c1-4(2)5(3-6)8-7/h4-6H,3H2,1-2H3
C5H11O3r_21 !! InChI=1S/C5H11O3/c1-4(2)5(3-6)8-7/h4-7H,1,3H2,2H3
C5H11O3r_15 !! InChI=1S/C5H11O3/c1-4(2)5(3-6)8-7/h5-7H,3H2,1-2H3

C5H1103r_37!! InChI=1S/C5H1103/c1-4(8-7)5(2,3)6/h4,6-7H,1H2,2-3H3
C5H1103r_46!! InChI=1S/C5H1103/c1-4(8-7)5(2,3)6/h4,6-7H,2H2,1,3H3
C5H1103r_40!! InChI=1S/C5H1103/c1-4(8-7)5(2,3)6/h4,6H,1-3H3
C5H1103r_42!! InChI=1S/C5H1103/c1-4(8-7)5(2,3)6/h4,7H,1-3H3
C5H1103r_36!! InChI=1S/C5H1103/c1-5(2,6)3-4-8-7/h3,6-7H,4H2,1-2H3
C5H1103r_48!! InChI=1S/C5H1103/c1-5(2,6)3-4-8-7/h6-7H,1,3-4H2,2H3
C5H1103r_39!! InChI=1S/C5H1103/c1-5(2,6)3-4-8-7/h6H,3-4H2,1-2H3
C5H1103r_6!! InChI=1S/C5H1103/c1-5(2,8-7)3-4-6/h3,6-7H,4H2,1-2H3
C5H1103r_7!! InChI=1S/C5H1103/c1-5(2,8-7)3-4-6/h4,6-7H,3H2,1-2H3
C5H1103r_2!! InChI=1S/C5H1103/c1-5(2,8-7)3-4-6/h6-7H,1,3-4H2,2H3
C5H1103r_5!! InChI=1S/C5H1103/c1-5(2,8-7)3-4-6/h6H,3-4H2,1-2H3
C5H1103r_9!! InChI=1S/C5H1103/c1-5(2-3-6)4-8-7/h2,5-7H,3-4H2,1H3
C5H1103r_10!! InChI=1S/C5H1103/c1-5(2-3-6)4-8-7/h3,5-7H,2,4H2,1H3
C5H1103r_4!! InChI=1S/C5H1103/c1-5(2-3-6)4-8-7/h5-6H,2-4H2,1H3
C5H1103r_8!! InChI=1S/C5H1103/c1-5(2-3-6)4-8-7/h5-7H,1-4H2
C5H1103r!! InChI=1S/C5H1103/c1-5(2-3-6)4-8-7/h6-7H,2-4H2,1H3
C5H1104r_6!! InChI=1S/C5H1104/c1-5(2,7)4(3-6)9-8/h3-4,6-8H,1-2H3
C5H1104r_5!! InChI=1S/C5H1104/c1-5(2,7)4(3-6)9-8/h4,6,8H,3H2,1-2H3
C5H1104r_1!! InChI=1S/C5H1104/c1-5(2,7)4(3-6)9-8/h4,6-7H,3H2,1-2H3
C5H1104r_7!! InChI=1S/C5H1104/c1-5(2,7)4(3-6)9-8/h4,6-8H,1,3H2,2H3
C5H1104r_3!! InChI=1S/C5H1104/c1-5(2,7)4(3-6)9-8/h4,7-8H,3H2,1-2H3
C5H1104r_21!! InChI=1S/C5H1104/c1-5(2,9-8)4(7)3-6/h3-4,6-8H,1-2H3
C5H1104r_13!! InChI=1S/C5H1104/c1-5(2,9-8)4(7)3-6/h4,6,8H,3H2,1-2H3
C5H1104r_18!! InChI=1S/C5H1104/c1-5(2,9-8)4(7)3-6/h4,6-7H,3H2,1-2H3
C5H1104r_16!! InChI=1S/C5H1104/c1-5(2,9-8)4(7)3-6/h4,6-8H,1,3H2,2H3
C5H1105r_32!! InChI=1S/C5H1105/c1-3(2)4(9-7)5(6)10-8/h3-5,7-8H,1-2H3
C5H1105r_37!! InChI=1S/C5H1105/c1-3(2)4(9-7)5(6)10-8/h3-6,8H,1-2H3
C5H1105r_39!! InChI=1S/C5H1105/c1-3(2)4(9-7)5(6)10-8/h3-7H,1-2H3
C5H1105r_25!! InChI=1S/C5H1105/c1-4(3-9-7)2-5(6)10-8/h4-6,8H,2-3H2,1H3
C5H1105r_16!! InChI=1S/C5H1105/c1-4(3-9-7)2-5(6)10-8/h4-7H,2-3H2,1H3
C5H1105r_20!! InChI=1S/C5H1105/c1-4(3-9-7)5(2-6)10-8/h4-5,7-8H,2-3H2,1H3
C5H1105r_42!! InChI=1S/C5H1105/c1-4(3-9-7)5(2-6)10-8/h4-6,8H,2-3H2,1H3
C5H1105r_6!! InChI=1S/C5H1105/c1-4(3-9-7)5(2-6)10-8/h4-7H,2-3H2,1H3
C5H1105r_3!! InChI=1S/C5H1105/c1-5(10-8,2-3-6)4-9-7/h6,8H,2-4H2,1H3
C5H1105r_10!! InChI=1S/C5H1105/c1-5(10-8,2-3-6)4-9-7/h6-7H,2-4H2,1H3
C5H1105r_13!! InChI=1S/C5H1105/c1-5(2,10-8)3-4(6)9-7/h4,6,8H,3H2,1-2H3
C5H1105r_29!! InChI=1S/C5H1105/c1-5(2,10-8)3-4(6)9-7/h4,6-7H,3H2,1-2H3
C5H1105r_9!! InChI=1S/C5H1105/c1-5(2,10-8)4(3-6)9-7/h4,6,8H,3H2,1-2H3
C5H1105r_47!! InChI=1S/C5H1105/c1-5(2,10-8)4(3-6)9-7/h4,6-7H,3H2,1-2H3
C5H1105r_18!! InChI=1S/C5H1105/c1-5(2,10-8)4(3-6)9-7/h4,7-8H,3H2,1-2H3
C5H1105r_2!! InChI=1S/C5H1105/c6-2-1-5(3-9-7)4-10-8/h5-7H,1-4H2
C5H120!! InChI=1S/C5H120/c1-5(2)3-4-6/h5-6H,3-4H2,1-2H3
C5H30!! InChI=1S/C5H30/c6-5-3-1-2-4-5/h1,3-4H
C5H40!! InChI=1S/C5H40/c6-5-3-1-2-4-5/h1-4H
C5H5!! InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H
C#CC*CCJ!! InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2
CJ*CC*CC*O!! InChI=1S/C5H5O/c1-2-3-4-5-6/h1-5H
C*CC*CCJ*O!! InChI=1S/C5H5O/c1-2-3-4-5-6/h2-4H,1H2
C5H4OH!! InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-4,6H
C5H5O!! InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-5H
C5H6!! InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2
C5H6-L!! InChI=1S/C5H6/c1-3-5-4-2/h1,4-5H,2H3
C5H6O_Olef_1!! InChI=1S/C5H6O/c1-2-3-4-5-6/h2-5H,1H2
C5H6O_Olef_3!! InChI=1S/C5H6O/c1-3-5(2)4-6/h3-4H,1-2H2
C5H6O_Olef!! InChI=1S/C5H6O/c1-3-5(6)4-2/h3-4H,1-2H2
Ccy(C*COCC*O)!! InChI=1S/C5H6O/c1-5-2-3-6-4-5/h2-4H,1H3
C5H5OH!! InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1-6H

C5H6O2_olef_3 !! InChI=1S/C5H6O2/c1-4(2)5(7)3-6/h3H,1H2,2H3
C5H6O2_olef_1 !! InChI=1S/C5H6O2/c1-5(4-7)2-3-6/h2-4H,1H3
C5H6O2_olef!! InChI=1S/C5H6O2/c1-5(4-7)2-3-6/h3-4H,1-2H2
C5H6O3_olef!! InChI=1S/C5H6O3/c1-4(3-6)2-5(7)8/h2-3H,1H3,(H,7,8)
C5H7 !! InChI=1S/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2
C*CC*CCJ !! InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2
C*CCJC*C !! InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2 - same as C*CC*CCJ
C5H7r_olef_1 !! InChI=1S/C5H7/c1-3-5-4-2/h4-5H,1H2,2H3
C5H7r_olef !! InChI=1S/C5H7/c1-3-5-4-2/h5H,1-3H2
B13DE2MJ !! InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2
C5H7Or_olef_1 !! InChI=1S/C5H7O/c1-2-3-4-5-6/h2-4H,1,5H2
C*CCJC*COH !! InChI=1S/C5H7O/c1-2-3-4-5-6/h2-6H,1H2
C5H7Or_olef_3 !! InChI=1S/C5H7O/c1-3-5(2)4-6/h3H,1-2,4H2
C5H7Or_olef!! InChI=1S/C5H7O/c1-3-5(6)4-2/h3-5H,1-2H2
C*(C)CCJ*(O) !! InChI=1S/C5H7O/c1-5(2)3-4-6/h1,3H2,2H3
CC(CJ)*CC*(O) !! InChI=1S/C5H7O/c1-5(2)3-4-6/h3-4H,1H2,2H3
CC(C)*CCJ*(O) !! InChI=1S/C5H7O/c1-5(2)3-4-6/h3H,1-2H3
C*(C)CJCC*O!! InChI=1S/C5H7O/c1-5(2)3-4-6/h4H,1-3H2
Ccy(CJCOC*C) !! InChI=1S/C5H7O/c1-5-2-3-6-4-5/h2-3H,4H2,1H3
C5H7O2r_olef_4 !! InChI=1S/C5H7O2/c1-4(2)5(7)3-6/h3,5H,1H2,2H3
C5H7O2r_olef_1 !! InChI=1S/C5H7O2/c1-5(4-7)2-3-6/h2-3H,4H2,1H3
C5H7O2r_olef !! InChI=1S/C5H7O2/c1-5(4-7)2-3-6/h3H,1-2,4H2
OC5H7O !! InChI=1S/C5H7O2/c6-4-2-1-3-5(4)7/h4H,1-3H2
C5H7O3r_olef_1 !! InChI=1S/C5H7O3/c1-4(3-6)2-5(7)8/h2-3,5,7H,1H3
C5H7O3r_olef_4 !! InChI=1S/C5H7O3/c1-4(3-6)2-5(7)8/h2H,3H2,1H3,(H,7,8)
C*CCC*C !! InChI=1S/C5H8/c1-3-5-4-2/h3-4H,1-2,5H2
C*CC*CC !! InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3
C5H8_olef !! InChI=1S/C5H8/c1-3-5-4-2/h5H,1,4H2,2H3
B12DE3M !! InChI=1S/C5H8/c1-4-5(2)3/h1H2,2-3H3
B13DE2M !! InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3
C*CC*CCOH !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2-4,6H,1,5H2
C5H8O_olef(m14) !! InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3
C5H8O_olef_4 !! InChI=1S/C5H8O/c1-3-4-5(2)6/h3-4H,1-2H3
C5H8O_olef_7 !! InChI=1S/C5H8O/c1-3-5(2)4-6/h3-4H,1-2H3
C5H8O_olef_5 !! InChI=1S/C5H8O/c1-3-5(2)4-6/h4H,2-3H2,1H3
C5H8O_olef_2 !! InChI=1S/C5H8O/c1-3-5(6)4-2/h3H,1,4H2,2H3
C5H8O_olef_8 !! InChI=1S/C5H8O/c1-4(2)5(3)6/h1H2,2-3H3
C5H8O_olef_1 !! InChI=1S/C5H8O/c1-5(2)3-4-6/h3-4,6H,1H2,2H3
CC(C)*CC*O !! InChI=1S/C5H8O/c1-5(2)3-4-6/h3-4H,1-2H3
IC4H7CHO !! InChI=1S/C5H8O/c1-5(2)3-4-6/h4H,1,3H2,2H3
C5H8O2_olef(m0) !! InChI=1S/C5H8O2/c1-2-3-4-5-7-6/h2-4,6H,1,5H2
C5H8O2_olef_13 !! InChI=1S/C5H8O2/c1-3(2)4-5(6)7-4/h4-6H,1H2,2H3
C*(C)C(C)C*O !! InChI=1S/C5H8O2/c1-3-5(2)4-7-6/h3,6H,1-2,4H2
C5H8O2_olef_2m !! InChI=1S/C5H8O2/c1-3-5(4-2)7-6/h3-6H,1-2H2
C5H8O2_olef!! InChI=1S/C5H8O2/c1-4(2)3-5(6)7/h3H,1-2H3,(H,6,7)
C5H8O2_olef_3 !! InChI=1S/C5H8O2/c1-4(2)5(7)3-6/h6H,1,3H2,2H3
C5H8O2_olef_8 !! InChI=1S/C5H8O2/c1-4-2-5(6)7-3-4/h2,5-6H,3H2,1H3
C5H8O2_olef_5 !! InChI=1S/C5H8O2/c1-5(2-3-6)4-7-5/h2-3,6H,4H2,1H3
C5H8O2_olef_1 !! InChI=1S/C5H8O2/c1-5(4-7)2-3-6/h2,4,6H,3H2,1H3
C*(C*O)CCOH !! InChI=1S/C5H8O2/c1-5(4-7)2-3-6/h4,6H,1-3H2
C*(C)C(OOH)C*O !! InChI=1S/C5H8O3/c1-4(2)5(3-6)8-7/h3,5,7H,1H2,2H3
C5H8O3_olef!! InChI=1S/C5H8O3/c1-5(2-3-6)4-8-7/h2-3,7H,4H2,1H3
C5H8O3_olef_4 !! InChI=1S/C5H8O3/c1-5(2-3-6)4-8-7/h3,7H,1-2,4H2
C5H8O4_olef_2 !! InChI=1S/C5H8O4/c1-4(3-6)2-5(7)9-8/h2-3,5,7-8H,1H3
C5H8O4_olef_4 !! InChI=1S/C5H8O4/c1-4(3-9-8)2-5(6)7/h2,8H,3H2,1H3,(H,6,7)
C*CCJCC !! InChI=1S/C5H9/c1-3-5-4-2/h3,5H,1,4H2,2H3

C*CCCJC !! InChI=1S/C5H9/c1-3-5-4-2/h3-4H,1,5H2,2H3
C5H9r_Olef_2 !! InChI=1S/C5H9/c1-3-5-4-2/h3-5H,1-2H3
C*CCCCJ !! InChI=1S/C5H9/c1-3-5-4-2/h3H,1-2,4-5H2
C5H9r_Olef_3 !! InChI=1S/C5H9/c1-3-5-4-2/h4-5H,1,3H2,2H3
AC5H9-D !! InChI=1S/C5H9/c1-4-5(2)3/h1-2,4H2,3H3
AC5H9-A2 !! InChI=1S/C5H9/c1-4-5(2)3/h2-4H2,1H3
CC5H9-A !! InChI=1S/C5H9/c1-4-5(2)3/h4-5H,1-2H2,3H3
B1E3M3J !! InChI=1S/C5H9/c1-4-5(2)3/h4H,1H2,2-3H3
AC5H9-C !! InChI=1S/C5H9/c1-4-5(2)3/h4H,2H2,1,3H3
C5H9Or_Olef_32 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h2,4,6H,1,3,5H2
C5H9Or_Olef_23 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h2,5-6H,1,3-4H2
C5H9Or_Olef_19 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h2-3,6H,1,4-5H2
C5H9Or_Olef_5m3 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h2-4,6H,5H2,1H3
C5H9Or_Olef_24 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h3-4H,2,5H2,1H3
C5H9Or_Olef_20 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h3-6H,2H2,1H3
C5H9Or_Olef_22 !! InChI=1S/C5H9O/c1-2-3-4-5-6/h4-6H,1-3H2
C5H9Or_Olef_14 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h3,5-6H,1-2,4H2
C5H9Or_Olef_15 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h3-4,6H,1-2H3
C5H9Or_Olef_29 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h3-5H,1-2H3
C5H9Or_Olef_10 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h3-6H,1H2,2H3
C5H9Or_Olef_9 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h3-6H,2H2,1H3
C5H9Or_Olef_16 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h4,6H,2-3H2,1H3
C5H9Or_Olef_17 !! InChI=1S/C5H9O/c1-3-4-5(2)6/h6H,1-4H2
C5H9Or_Olef_44 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h2-4H2,1H3
C5H9Or_Olef_2m !! InChI=1S/C5H9O/c1-3-5(2)4-6/h3,6H,1,4H2,2H3
C5H9Or_Olef_33 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h3,6H,2,4H2,1H3
C5H9Or_Olef_34 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h3-4,6H,1-2H3
B2E2M1OJ !! InChI=1S/C5H9O/c1-3-5(2)4-6/h3H,4H2,1-2H3
C5H9Or_Olef_37 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h4,6H,1,3H2,2H3
C5H9Or_Olef_35 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h4,6H,2-3H2,1H3
TC4H8CHO !! InChI=1S/C5H9O/c1-3-5(2)4-6/h4-5H,2-3H2,1H3
C5H9Or_Olef_38 !! InChI=1S/C5H9O/c1-3-5(2)4-6/h6H,1-4H2
C5H9Or_Olef_26 !! InChI=1S/C5H9O/c1-3-5(6)4-2/h3,5H,1,4H2,2H3
C5H9Or_Olef_13 !! InChI=1S/C5H9O/c1-3-5(6)4-2/h3-6H,1H2,2H3
C5H9Or_Olef_1m !! InChI=1S/C5H9O/c1-4(2)5(3)6/h5-6H,1,3H2,2H3
C5H9Or_Olef_41 !! InChI=1S/C5H9O/c1-4(2)5(3)6/h5-6H,1-2H2,3H3
AC5H9O-C !! InChI=1S/C5H9O/c1-4(2)5(3)6/h5H,1H2,2-3H3
C5H9Or_Olef_40 !! InChI=1S/C5H9O/c1-4(2)5(3)6/h6H,1H2,2-3H3
C5H9Or_Olef_42 !! InChI=1S/C5H9O/c1-4(2)5(3)6/h6H,3H2,1-2H3
C5H9Or_Olef_4 !! InChI=1S/C5H9O/c1-4-5(2,3)6/h4,6H,1-2H2,3H3
B1E3M3OJ !! InChI=1S/C5H9O/c1-4-5(2,3)6/h4H,1H2,2-3H3
C*(C)CJCOH!! InChI=1S/C5H9O/c1-5(2)3-4-6/h3,6H,1,4H2,2H3
CC(C)*CCJOH!! InChI=1S/C5H9O/c1-5(2)3-4-6/h3-4,6H,1-2H3
C5H9Or_2 !! InChI=1S/C5H9O/c1-5(2)3-4-6/h3-5H,1-2H3
C5H9Or_Olef_1 !! InChI=1S/C5H9O/c1-5(2)3-4-6/h3-6H,1H2,2H3
B2E3M1OJ !! InChI=1S/C5H9O/c1-5(2)3-4-6/h3H,4H2,1-2H3
CC(C)*CCOJ !! InChI=1S/C5H9O/c1-5(2)3-4-6/h3H,4H2,1-2H3
C*(C)CCJOH!! InChI=1S/C5H9O/c1-5(2)3-4-6/h4,6H,1,3H2,2H3
C5H9Or !! InChI=1S/C5H9O/c1-5(2)3-4-6/h4-5H,1,3H2,2H3
CCJ(C)CC*O !! InChI=1S/C5H9O/c1-5(2)3-4-6/h4H,3H2,1-2H3
CC(C)CCJ(*O) !! InChI=1S/C5H9O/c1-5(2)3-4-6/h5H,3H2,1-2H3
C*(C)CJCCOH!! InChI=1S/C5H9O/c1-5(2)3-4-6/h6H,1-4H2
C5H9O2r_Olef_1 !! InChI=1S/C5H9O2/c1-4(2)3-5(6)7/h3,5-6H,1-2H3
C5H9O2r_1 !! InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h3,5,7H,1-2H3
C5H9O2r_3 !! InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h3-5H,1-2H3
C5H9O2r_Olef_4 !! InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h5-6H,1,3H2,2H3
C5H9O2r_Olef_7 !! InChI=1S/C5H9O2/c1-5(2,7)3-4-6/h3-4,6H,1-2H3
C5H9O2r_2(m0) !! InChI=1S/C5H9O2/c1-5(2,7)3-4-6/h3-4,7H,1-2H3

C5H9O2r_2 !! InChI=1S/C5H9O2/c1-5(2,7)3-4-6/h4H,3H2,1-2H3
C5H9O2r_Olef_3 !! InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h2,6H,3-4H2,1H3
C5H9O2r !! InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h3,5H,2,4H2,1H3
C*(C(COJ)CCOH) !! InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h6H,1-4H2
C5H9O3r_Olef_80 !! InChI=1S/C5H9O3/c1-2-3-4-5(6)8-7/h2,5-6H,1,3-4H2
C5H9O3r_Olef_67 !! InChI=1S/C5H9O3/c1-2-3-4-5(6)8-7/h3-6H,2H2,1H3
C5H9O3r_Olef_87 !! InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h2,5,7H,1,3-4H2
C5H9O3r_Olef_86 !! InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h2,5-6H,1,3-4H2
C5H9O3r_Olef_84 !! InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h2-3,5,7H,4H2,1H3
C5H9O3r_Olef_60 !! InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h2-3,5-6H,4H2,1H3
C5H9O3r_Olef_38 !! InChI=1S/C5H9O3/c1-2-3-5(6)4-8-7/h2,5,7H,1,3-4H2
C5H9O3r_Olef_37 !! InChI=1S/C5H9O3/c1-2-3-5(6)4-8-7/h2,5-6H,1,3-4H2
C5H9O3r_Olef_51 !! InChI=1S/C5H9O3/c1-2-3-5(6)4-8-7/h2-3,5,7H,4H2,1H3
C5H9O3r_Olef_56 !! InChI=1S/C5H9O3/c1-2-3-5(6)4-8-7/h2-3,5-6H,4H2,1H3
C5H9O3r_Olef_32 !! InChI=1S/C5H9O3/c1-2-3-5(6)4-8-7/h3,6H,2,4H2,1H3
C5H9O3r_Olef_112 !! InChI=1S/C5H9O3/c1-2-5(3-6)4-8-7/h2,6H,3-4H2,1H3
C5H9O3r_Olef_106 !! InChI=1S/C5H9O3/c1-2-5(3-6)4-8-7/h3,6H,2,4H2,1H3
C5H9O3r_Olef_78 !! InChI=1S/C5H9O3/c1-2-5(8-7)3-4-6/h2,5-6H,1,3-4H2
C5H9O3r_Olef_71 !! InChI=1S/C5H9O3/c1-2-5(8-7)3-4-6/h3-6H,2H2,1H3
C5H9O3r_11 !! InChI=1S/C5H9O3/c1-3(2)4(6)5(7)8/h3,5,7H,1-2H3
C5H9O3r_10 !! InChI=1S/C5H9O3/c1-3(2)4(6)5(7)8/h3-4H,1-2H3,(H,7,8)
C5H9O3r_Olef_99 !! InChI=1S/C5H9O3/c1-3-4(2)5(6)8-7/h3,5-6H,1-2H3
C5H9O3r_Olef_108 !! InChI=1S/C5H9O3/c1-3-4(2)5(6)8-7/h5-6H,2-3H2,1H3
C5H9O3r_Olef_24 !! InChI=1S/C5H9O3/c1-3-4-5(2,6)8-7/h3-4,6H,1-2H3
C5H9O3r_Olef_93 !! InChI=1S/C5H9O3/c1-3-5(2,4-6)8-7/h3,6H,1,4H2,2H3
C5H9O3r_Olef_117 !! InChI=1S/C5H9O3/c1-3-5(2,4-6)8-7/h3,7H,1,4H2,2H3
C5H9O3r_Olef_89 !! InChI=1S/C5H9O3/c1-3-5(2,6)4-8-7/h3,6H,1,4H2,2H3
C5H9O3r_Olef_90 !! InChI=1S/C5H9O3/c1-3-5(2,6)4-8-7/h3,7H,1,4H2,2H3
C5H9O3r_Olef_17 !! InChI=1S/C5H9O3/c1-3-5(6)4(2)8-7/h3-5,7H,1H2,2H3
C5H9O3r_Olef_13m !! InChI=1S/C5H9O3/c1-3-5(6)4(2)8-7/h3-6H,1H2,2H3
C5H9O3r_Olef_40 !! InChI=1S/C5H9O3/c1-3-5(8-7)4(2)6/h3-5,7H,1H2,2H3
C5H9O3r_Olef_45 !! InChI=1S/C5H9O3/c1-3-5(8-7)4(2)6/h3-6H,1H2,2H3
C5H9O3r_Olef_35 !! InChI=1S/C5H9O3/c1-3-5(8-7)4(2)6/h5-6H,2-3H2,1H3
C5H9O3r_Olef_3 !! InChI=1S/C5H9O3/c1-4(2)3-5(6)8-7/h3,5-6H,1-2H3
C5H9O3r_Olef_13 !! InChI=1S/C5H9O3/c1-4(2)3-5(6)8-7/h3,5-7H,1H2,2H3
C5H9O3r_Olef !! InChI=1S/C5H9O3/c1-4(2)3-5(6)8-7/h5-6H,1,3H2,2H3
C5H9O3r_Olef_121 !! InChI=1S/C5H9O3/c1-4(2)5(3,6)8-7/h6H,1H2,2-3H3
C5H9O3r_Olef_12 !! InChI=1S/C5H9O3/c1-4(2)5(3-6)8-7/h5,7H,1,3H2,2H3
C5H9O3r_Olef_4 !! InChI=1S/C5H9O3/c1-4(2)5(3-6)8-7/h5-6H,1,3H2,2H3
C5H9O3r_Olef_128 !! InChI=1S/C5H9O3/c1-4(2)5(6)3-8-7/h5,7H,1,3H2,2H3
C5H9O3r_Olef_129 !! InChI=1S/C5H9O3/c1-4(2)5(6)3-8-7/h5-6H,1,3H2,2H3
C5H9O3r_Olef_124 !! InChI=1S/C5H9O3/c1-4(2)5(6)3-8-7/h6H,3H2,1-2H3
C5H9O3r_13 !! InChI=1S/C5H9O3/c1-4(2-6)5(8)3-7/h4,7H,2-3H2,1H3
C5H9O3r !! InChI=1S/C5H9O3/c1-4(3-6)2-5(7)8/h3-5,7H,2H2,1H3
C5H9O3r_7 !! InChI=1S/C5H9O3/c1-4(3-6)2-5(7)8/h4H,2-3H2,1H3,(H,7,8)
C5H9O3r_Olef_103 !! InChI=1S/C5H9O3/c1-4(3-6)5(2)8-7/h3,5-6H,1-2H3
C5H9O3r_Olef_115 !! InChI=1S/C5H9O3/c1-4(3-6)5(2)8-7/h5-6H,1,3H2,2H3
C5H9O3r_Olef_119 !! InChI=1S/C5H9O3/c1-4(3-8-7)5(2)6/h5-6H,1,3H2,2H3
C5H9O3r_Olef_123 !! InChI=1S/C5H9O3/c1-4(3-8-7)5(2)6/h6H,3H2,1-2H3
C5H9O3r_Olef_29 !! InChI=1S/C5H9O3/c1-4(6)3-5(2)8-7/h3,5-6H,1-2H3
C5H9O3r_Olef_125 !! InChI=1S/C5H9O3/c1-4(6)5(2,3)8-7/h6H,1H2,2-3H3
C5H9O3r_8 !! InChI=1S/C5H9O3/c1-5(2,8)3-4(6)7/h3H2,1-2H3,(H,6,7)
C5H9O3r_15 !! InChI=1S/C5H9O3/c1-5(2,8)4(7)3-6/h6H,3H2,1-2H3
C5H9O3r_Olef_7 !! InChI=1S/C5H9O3/c1-5(2,8-7)3-4-6/h3-4,6H,1-2H3
C5H9O3r_Olef_8 !! InChI=1S/C5H9O3/c1-5(2-3-6)4-8-7/h2,6H,3-4H2,1H3
C5H9O3r_Olef_10 !! InChI=1S/C5H9O3/c1-5(2-3-6)4-8-7/h2-3,6-7H,4H2,1H3
C*(C(COOJ)CCOH) !! InChI=1S/C5H9O3/c1-5(2-3-6)4-8-7/h6H,1-4H2
C5H9O3r_Olef_95 !! InChI=1S/C5H9O3/c1-5(4-6)2-3-8-7/h2,6H,3-4H2,1H3

C5H9O3r_Olef_111 !! InChI=1S/C5H9O3/c1-5(4-6)2-3-8-7/h4,6H,2-3H2,1H3
C5H9O3r_Olef_109 !! InChI=1S/C5H9O3/c1-5(4-6)2-3-8-7/h6H,1-4H2
C5H9O3r_Olef_47 !! InChI=1S/C5H9O3/c1-5(6)3-2-4-8-7/h2-3,5-6H,4H2,1H3
C5H9O3r_Olef_36 !! InChI=1S/C5H9O3/c1-5(6)3-2-4-8-7/h6H,1-4H2
C5H9O3r_4 !! InChI=1S/C5H9O3/c1-5(8,4-7)2-3-6/h4,6H,2-3H2,1H3
C5H9O3r_Olef_63 !! InChI=1S/C5H9O3/c1-5(8-7)3-2-4-6/h2-3,5-6H,4H2,1H3
C5H9O3r_Olef_75 !! InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h1,3,6H,2,4-5H2
C5H9O3r_Olef_73 !! InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h2,4,6H,1,3,5H2
O2C4H8CHO !! InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h4H,1-3,5H2
O2HC4H8CO !! InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h7H,1-3,5H2
C5H9O5r_Olef_13 !! InChI=1S/C5H9O5/c1-3(2)4(9-7)5(6)10-8/h4-5,7-8H,1H2,2H3
C5H9O5r_Olef_18 !! InChI=1S/C5H9O5/c1-3(2)4(9-7)5(6)10-8/h4-6,8H,1H2,2H3
C5H9O5r_Olef_9 !! InChI=1S/C5H9O5/c1-4(3-9-7)2-5(6)10-8/h2,5-6,8H,3H2,1H3
C5H9O5r_Olef_3 !! InChI=1S/C5H9O5/c1-4(3-9-7)2-5(6)10-8/h2,5-7H,3H2,1H3
C5H9O5r_Olef_7 !! InChI=1S/C5H9O5/c1-5(10-8,2-3-6)4-9-7/h2-3,6-7H,4H2,1H3
C6H10 !! InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2
B13DE2E !! InChI=1S/C6H10/c1-4-6(3)5-2/h4H,1,3,5H2,2H3
C6H11r_Olef_5 !! InChI=1S/C6H11/c1-3-5-6-4-2/h3,5-6H,4H2,1-2H3
C6H11r_Olef_13 !! InChI=1S/C6H11/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3
C*CCCCJC !! InChI=1S/C6H11/c1-3-5-6-4-2/h3-4H,1,5-6H2,2H3
C*CCCCJ !! InChI=1S/C6H11/c1-3-5-6-4-2/h3H,1-2,4-6H2
C6H11r_Olef_15 !! InChI=1S/C6H11/c1-4-5-6(2)3/h4,6H,1-2,5H2,3H3
C6H11r_Olef_10 !! InChI=1S/C6H11/c1-4-5-6(2)3/h4-6H,1H2,2-3H3
C6H11r_Olef_9 !! InChI=1S/C6H11/c1-4-5-6(2)3/h4-6H,2H2,1,3H3
C6H11r_Olef!! InChI=1S/C6H11/c1-4-5-6(2)3/h5H,2,4H2,1,3H3
C6H11r_Olef_1 !! InChI=1S/C6H11/c1-4-6(3)5-2/h1,3-5H2,2H3
C6H11r_Olef_(m1) !! InChI=1S/C6H11/c1-4-6(3)5-2/h4,6H,1,3,5H2,2H3
C6H11r_Olef_11 !! InChI=1S/C6H11/c1-4-6(3)5-2/h4-6H,1H2,2-3H3
C6H11r_Olef_3 !! InChI=1S/C6H11/c1-4-6(3)5-2/h4H,1,5H2,2-3H3
C6H11r_Olef(m0) !! InChI=1S/C6H11/c1-4-6(3)5-2/h4H,3,5H2,1-2H3
C6H11r_Olef_2 !! InChI=1S/C6H11/c1-5(2)6(3)4/h5H,1,3H2,2,4H3
C6H11r_Olef_4 !! InChI=1S/C6H11/c1-5-6(2,3)4/h5H,1-2H2,3-4H3
C6H11Or !! InChI=1S/C6H11O/c1-5(2)6(3)4-7/h4,6H,1-3H3
C6H11Or_2 !! InChI=1S/C6H11O/c1-6(2,3)4-5-7/h4-5H,1-3H3
C6H13r !! InChI=1S/C6H13/c1-4-5-6(2)3/h5-6H,4H2,1-3H3
C6H13r_4 !! InChI=1S/C6H13/c1-4-6(3)5-2/h4,6H,5H2,1-3H3
C6H13r_7 !! InChI=1S/C6H13/c1-4-6(3)5-2/h4-5H2,1-3H3
C6H13r_1 !! InChI=1S/C6H13/c1-5(2)6(3)4/h5-6H,1H2,2-4H3
C6H13r_5 !! InChI=1S/C6H13/c1-5(2)6(3)4/h5H,1-4H3
C6H13r_8 !! InChI=1S/C6H13/c1-5-6(2,3)4/h2,5H2,1,3-4H3
C6H13r_6 !! InChI=1S/C6H13/c1-5-6(2,3)4/h5H,1-4H3
C6H13Or_1 !! InChI=1S/C6H13O/c1-5(2)6(3)4-7/h6-7H,4H2,1-3H3
CC(C)(C)CJOH !! InChI=1S/C6H13O/c1-6(2,3)4-5-7/h4,7H,5H2,1-3H3
C6H2 !! InChI=1S/C6H2/c1-3-5-6-4-2/h1-2H
C6H3 !! InChI=1S/C6H3/c1-3-5-6-4-2/h1-3H
P-C6H3O2 !! InChI=1S/C6H3O2/c7-5-1-2-6(8)4-3-5/h1-3H
C-C6H4 !! InChI=1S/C6H4/c1-2-4-6-5-3-1/h1-4H
L-C6H4 !! InChI=1S/C6H4/c1-3-5-6-4-2/h1-2,5-6H
P-C6H4O2 !! InChI=1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H
O-C6H4O2 !! InChI=1S/C6H4O2/c7-5-3-1-2-4-6(5)8/h1-4H
C6H5 !! InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H
C6H4OH !! InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-2,4-5,7H
C6H5O !! InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-5H

P-OC6H5OJ !! InChI=1S/C6H5O2/c7-5-1-2-6(8)4-3-5/h1-5H
OC6H4OH !! InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-4,7H
O-OC6H5OJ !! InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-5H
C6H5OO !! InChI=1S/C6H5O2/c7-8-6-4-2-1-3-5-6/h1-5H
C6H6 !! InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
C6H6_Olef !! InChI=1S/C6H6/c1-3-5-6-4-2/h5-6H,1-2H2
fulvene !! InChI=1S/C6H6/c1-6-4-2-3-5-6/h2-5H,1H2
C6H5OH !! InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H
C6H5OOH !! InChI=1S/C6H6O2/c7-8-6-4-2-1-3-5-6/h1-5,7H
C6H7r_Olef !! InChI=1S/C6H7/c1-3-5-6-4-2/h3,5-6H,1-2H2
C6H7r_Olef_1 !! InChI=1S/C6H7/c1-3-5-6-4-2/h5H,1-2,6H2
C6H8_Olef_1 !! InChI=1S/C6H8/c1-3-5-6-4-2/h3,6H,1-2,5H2
C6H8_Olef !! InChI=1S/C6H8/c1-4-6(3)5-2/h4-5H,1-3H2
C6H9-A !! InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2
C*JC*CC*C !! InChI=1S/C6H9/c1-3-5-6-4-2/h3H,1-2,5-6H2
C6H9r_Olef_4 !! InChI=1S/C6H9/c1-3-5-6-4-2/h4-5H,1,6H2,2H3
C6H9r_Olef_5 !! InChI=1S/C6H9/c1-3-5-6-4-2/h6H,1-3,5H2
C6H9r_Olef !! InChI=1S/C6H9/c1-4-6(3)5-2/h4-5H,1,3H2,2H3
C6H9r_Olef_2 !! InChI=1S/C6H9/c1-4-6(3)5-2/h4-5H,1-2H2,3H3
C6H9r_Olef_3 !! InChI=1S/C6H9/c1-4-6(3)5-2/h4-6H,1-3H2
C6H9r_Olef_1 !! InChI=1S/C6H9/c1-4-6(3)5-2/h4H,1-3,5H2
C7H10_Olef !! InChI=1S/C7H10/c1-4-5-6-7(2)3/h5H,1-2,6H2,3H3
H15DE2M-T !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h1-2,5-6H2,3H3
C7H11r_Olef_4 !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h4,6H,1-2,5H2,3H3
C7H11r_Olef_5 !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h4-5H,1-2,6H2,3H3
C7H11r_Olef_3 !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h4H,1-3,5-6H2
C7H11r_Olef_1 !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h5,7H,1-2,6H2,3H3
C7H11r_Olef !! InChI=1S/C7H11/c1-4-5-6-7(2)3/h5H,1,6H2,2-3H3
C*(C)CCC*C !! InChI=1S/C7H12/c1-4-5-6-7(2)3/h4H,1-2,5-6H2,3H3
C7H13r_Olef_1 !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h1-2,4-6H2,3H3
C7H13r_Olef_3 !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h4,7H,1-2,5-6H2,3H3
C7H13r_Olef_2 !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h4H,1,5-6H2,2-3H3
C7H13r_Olef !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h4H,2,5-6H2,1,3H3
C7H9r_Olef_1 !! InChI=1S/C7H9/c1-4-5-6-7(2)3/h5-6H,1-2H2,3H3
C7H9r_Olef !! InChI=1S/C7H9/c1-4-5-6-7(2)3/h5H,1-3,6H2
C8H10_Olef !! InChI=1S/C8H10/c1-4-6-7-8(3)5-2/h5-6H,1-3,7H2
C8H11r_Olef_1 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h4-5,7H,1-3,6H2
C8H11r_Olef !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h4-6H,1-3,7H2
C8H11r_Olef_6 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h5-6,8H,1-3,7H2
C8H11r_Olef_2 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h5-6H,1,3,7H2,2H3
C8H11r_Olef_4 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h5-6H,1-2,7H2,3H3
C8H11r_Olef_7 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h5H,1-3,6-7H2
C8H11r_Olef_3 !! InChI=1S/C8H11/c1-4-6-7-8(3)5-2/h6H,1-3,5,7H2
HX15DE2V !! InChI=1S/C8H12/c1-4-6-7-8(3)5-2/h4-5H,1-3,6-7H2
C8H13r_Olef_6 !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5,8H,1-3,6-7H2
C8H13r_Olef_2 !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5H,1,3,6-7H2,2H3
C8H13r_Olef_4 !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5H,1-2,6-7H2,3H3
C8H13r_Olef !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5H,2-3,6-7H2,1H3
C8H13r_Olef_3 !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4H,1-3,5-7H2
C8H13r_Olef_1 !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h5H,1-4,6-7H2
H15DE25DM-S !! InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h1-3,5-6H2,4H3
H15DE25DM-A !! InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3
H15DE25DM-AO !! InChI=1S/C8H13O/c1-6(2)5-8(9)7(3)4/h8H,1,3,5H2,2,4H3
H15DE25DM-SO !! InChI=1S/C8H13O/c1-7(2)4-5-8(3)6-9/h1,3-6H2,2H3
H15DE25DM !! InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3

IC4H7OOC4H7 !! InChI=1S/C8H14O2/c1-7(2)5-9-10-6-8(3)4/h1,3,5-6H2,2,4H3
 C8H9r_Olef !! InChI=1S/C8H9/c1-4-6-7-8(3)5-2/h5-7H,1-3H2
 C9H13r_Olef !! InChI=1S/C9H13/c1-5-9(4)7-6-8(2)3/h5,7H,1-2,4,6H2,3H3
 C9H13r_Olef_1 !! InChI=1S/C9H13/c1-5-9(4)7-6-8(2)3/h5-6H,1-2,4,7H2,3H3
 C9H13r_Olef_2 !! InChI=1S/C9H13/c1-5-9(4)7-6-8(2)3/h5H,1-4,6-7H2
 HX15DE2V5M !! InChI=1S/C9H14/c1-5-9(4)7-6-8(2)3/h5H,1-2,4,6-7H2,3H3
 C9H15r_Olef_1 !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h1-2,4-7H2,3H3
 C9H15r_Olef_4 !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h5,8H,1-2,4,6-7H2,3H3
 C9H15r_Olef_6 !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h5,9H,1-2,4,6-7H2,3H3
 C9H15r_Olef_2 !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h5H,1,4,6-7H2,2-3H3
 C9H15r_Olef_5 !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h5H,1-2,6-7H2,3-4H3
 C9H15r_Olef !! InChI=1S/C9H15/c1-5-9(4)7-6-8(2)3/h5H,2,4,6-7H2,1,3H3
 CH !! InChI=1S/CH/h1H
 CH* !! InChI=1S/CH/h1H - excited
 CH2 !! InChI=1S/CH2/h1H2
 CH2(S) !! InChI=1S/CH2/h1H2 - s
 HCOH !! InChI=1S/CH2O/c1-2/h1-2H
 CH2O !! InChI=1S/CH2O/c1-2/h1H2
 HOCHO !! InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)
 HO2CHO !! InChI=1S/CH2O3/c2-1-4-3/h1,3H
 CH3 !! InChI=1S/CH3/h1H3
 CH3O !! InChI=1S/CH3O/c1-2/h1H3
 CH2OH !! InChI=1S/CH3O/c1-2/h2H,1H2
 CH3O2 !! InChI=1S/CH3O2/c1-3-2/h1H3
 CH2O2H !! InChI=1S/CH3O2/c1-3-2/h2H,1H2
 HOCH2O !! InChI=1S/CH3O2/c2-1-3/h2H,1H2
 HOCH2O2 !! InChI=1S/CH3O3/c2-1-4-3/h2H,1H2
 OCH2O2H !! InChI=1S/CH3O3/c2-1-4-3/h3H,1H2
 CH4 !! InChI=1S/CH4/h1H4
 CH3OH !! InChI=1S/CH4O/c1-2/h2H,1H3
 CH3O2H !! InChI=1S/CH4O2/c1-3-2/h2H,1H3
 HOCH2O2H !! InChI=1S/CH4O3/c2-1-4-3/h2-3H,1H2
 HCO !! InChI=1S/CHO/c1-2/h1H
 HOCO !! InChI=1S/CHO2/c2-1-3/h(H,2,3)
 OCHO !! InChI=1S/CHO2/c2-1-3/h1H
 O2CHO !! InChI=1S/CHO3/c2-1-4-3/h1H
 CO !! InChI=1S/CO/c1-2
 CO2 !! InChI=1S/CO2/c2-1-3
 H !! InChI=1S/H
 H2 !! InChI=1S/H2/h1H
 H2O !! InChI=1S/H2O/h1H2
 H2O2 !! InChI=1S/H2O2/c1-2/h1-2H
 HE !! InChI=1S/He
 OH !! InChI=1S/HO/h1H
 OH* !! InChI=1S/HO/h1H - excited
 HO2 !! InChI=1S/HO2/c1-2/h1H
 N2 !! InChI=1S/N2/c1-2
 O !! InChI=1S/O
 O2 !! InChI=1S/O2/c1-2
 END

THERMO ALL

298.00 600.00 1000.0
 C*C(CJ)CC*O C 5 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 -6.30322350E-01 6.21604772E-02-5.72541246E-05 2.88288336E-08-5.88683075E-
 12 2
 2.39283921E+03 2.86080209E+01-6.30322350E-01 6.21604772E-02-5.72541246E-
 05 3
 2.88288336E-08-5.88683075E-12 2.39283921E+03 2.86080209E+01
 4
 C*C(C)C(OOH)C*O C 5 O 3 H 8 G 3E+02 1E+03 6E+02
 1
 4.92674196E+00 6.38297607E-02-7.14928214E-05 5.53607513E-08-1.94283000E-
 11 2
 -2.60269321E+04 7.21620681E+00 4.92674196E+00 6.38297607E-02-7.14928214E-
 05 3
 5.53607513E-08-1.94283000E-11-2.60269321E+04 7.21620681E+00
 4
 C*[C]CC*O C 4 O 1 H 5 G 3E+02 1E+03 6E+02
 1
 3.50553286E+00 2.40686238E-02 3.94476851E-06-2.08996352E-08 9.82215489E-
 12 2
 1.71210654E+04 1.41739218E+01 3.50553286E+00 2.40686238E-02 3.94476851E-
 06 3
 -2.08996352E-08 9.82215489E-12 1.71210654E+04 1.41739218E+01
 4
 H L 6/94H 1 0 0 0G 200.000 6000.00 1000.00
 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 2
 0.25473660E+05-0.44668285E+00 0.25000000E+01 0.00000000E+00
 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00 0.25473660E+05-0.44668285E+00
 0.26219035E+05 4
 H2 TPIS78H 2 0 0 0G 200.000 6000.00 1000.00
 1
 2.93286575E+00 8.26608026E-04-1.46402364E-07 1.54100414E-11-6.88804800E-
 16 2
 -8.13065581E+02-1.02432865E+00 2.34433112E+00 7.98052075E-03-1.94781510E-
 05 3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01
 0.00000000E+00 4
 O L 1/900 1 0 0 0G 200.000 6000.00 1000.00
 1
 2.54363697E+00-2.73162486E-05-4.19029520E-09 4.95481845E-12-4.79553694E-
 16 2
 2.92260120E+04 4.92229457E+00 3.16826710E+00-3.27931884E-03 6.64306396E-
 06 3
 -6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00
 2.99687009E+04 4
 O2 RUS 890 2 0 0 0G 200.000 6000.00 1000.00
 1
 3.66096065E+00 6.56365811E-04-1.41149627E-07 2.05797935E-11-1.29913436E-
 15 2
 -1.21597718E+03 3.41536279E+00 3.78245636E+00-2.99673416E-03 9.84730201E-
 06 3
 -9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00
 0.00000000E+00 4

OH IU3/03O 1 H 1 0 0G 200.000 6000.00 1000.00
 1
 2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-
 15 2
 3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-
 06 3
 -3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01
 4.48613328E+03 4
 OH* 121286O 1H 1 G 0300.00 5000.00 1000.00
 1
 0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-
 14 2
 5.02650000E+04 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-
 05 3
 0.02387202E-07-0.08431442E-11 5.00213000E+04 0.13588605E+01
 4
 H2O L 5/89H 2 O 1 0 0G 200.000 6000.00 1000.00
 1
 0.26770389E+01 0.29731816E-02-0.77376889E-06 0.94433514E-10-0.42689991E-
 14 2
 -0.29885894E+05 0.68825500E+01 0.41986352E+01-0.20364017E-02 0.65203416E-
 05 3
 -0.54879269E-08 0.17719680E-11-0.30293726E+05-0.84900901E+00-
 0.29084817E+05 4
 N2 G 8/02N 2 0 0 0G 200.000 6000.00 1000.00
 1
 2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-
 15 2
 -9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-
 07 3
 2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00
 0.00000000E+00 4
 HO2 T 1/09H 1O 2 0 0G 200.000 5000.00 1000.00
 1
 4.17228741E+00 1.88117627E-03-3.46277286E-07 1.94657549E-11 1.76256905E-
 16 2
 3.10206839E+01 2.95767672E+00 4.30179807E+00-4.74912097E-03 2.11582905E-
 05 3
 -2.42763914E-08 9.29225225E-12 2.64018485E+02 3.71666220E+00
 1.47886045E+03 4
 H2O2 T 8/03H 2O 2 0 0G 200.000 6000.00 1000.00
 1
 4.57977305E+00 4.05326003E-03-1.29844730E-06 1.98211400E-10-1.13968792E-
 14 2
 -1.80071775E+04 6.64970694E-01 4.31515149E+00-8.47390622E-04 1.76404323E-
 05 3
 -2.26762944E-08 9.08950158E-12-1.77067437E+04 3.27373319E+00-
 1.63425145E+04 4
 AR G 5/97AR 1 0 0 0G 200.000 6000.00 1000.00
 1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 2
 -7.45375000E+02 4.37967491E+00 2.50000000E+00 0.00000000E+00
 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 4.37967491E+00
 0.00000000E+00 4
 CH2O T 5/11H 2C 1O 1 0G 200.000 6000.00 1000.00
 1

3.16952665E+00 6.19320560E-03-2.25056366E-06 3.65975660E-10-2.20149458E-
 14 2
 -1.45486831E+04 6.04207898E+00 4.79372312E+00-9.90833322E-03 3.73219990E-
 05 3
 -3.79285237E-08 1.31772641E-11-1.43791953E+04 6.02798058E-01-
 1.31293365E+04 4
 CO RUS 79C 1O 1 0 0G 200.000 6000.00 1000.00
 1
 0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-
 14 2
 -0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-
 05 3
 0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-
 0.13293628E+05 4
 CO2 L 7/88C 1O 2 0 0G 200.000 6000.00 1000.00
 1
 0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-
 14 2
 -0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-
 05 3
 0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-
 0.47328105E+05 4
 HCO T 5/03C 1H 1O 1 0G 200.000 6000.00 1000.00
 1
 3.92001542E+00 2.52279324E-03-6.71004164E-07 1.05615948E-10-7.43798261E-
 15 2
 3.65342928E+03 3.58077056E+00 4.23754610E+00-3.32075257E-03 1.40030264E-
 05 3
 -1.34239995E-08 4.37416208E-12 3.87241185E+03 3.30834869E+00
 5.08749163E+03 4
 HO2CHO 6/26/95 THERMC 1H 2O 3 0G 300.000 5000.000 1378.00
 21
 9.87503878E+00 4.64663708E-03-1.67230522E-06 2.68624413E-10-1.59595232E-
 14 2
 -3.80502496E+04-2.24939155E+01 2.42464726E+00 2.19706380E-02-1.68705546E-
 05 3
 6.25612194E-09-9.11645843E-13-3.54828006E+04 1.75027796E+01
 4
 O2CHO 6/26/95 THERMC 1H 1O 3 0G 300.000 5000.000 1368.00
 11
 7.24075139E+00 4.63312951E-03-1.63693995E-06 2.59706693E-10-1.52964699E-
 14 2
 -1.87027618E+04-6.49547212E+00 3.96059309E+00 1.06002279E-02-5.25713351E-
 06 3
 1.01716726E-09-2.87487602E-14-1.73599383E+04 1.17807483E+01
 4
 HOCHO L 8/88H 2C 1O 2 0G 200.000 6000.00 1000.00
 1
 0.46138316E+01 0.64496364E-02-0.22908251E-05 0.36716047E-09-0.21873675E-
 13 2
 -0.47514850E+05 0.84788383E+00 0.38983616E+01-0.35587795E-02 0.35520538E-
 04 3
 -0.43849959E-07 0.17107769E-10-0.46770609E+05 0.73495397E+01-
 0.45531246E+05 4
 HOCO T05/06H 1C 1O 2 0G 200.000 6000.00
 1000.00 1
 5.39206152E+00 4.11221455E-03-1.48194900E-06 2.39875460E-10-1.43903104E-
 14 2

-2.38606717E+04-2.23529091E+00 2.92207919E+00 7.62453859E-03 3.29884437E-
 06 3
 -1.07135205E-08 5.11587057E-12-2.30281524E+04 1.12925886E+01-
 2.18076591E+04 4
 OCHO ATCT/AC 1 O 2 H 1 0 G 200.000 6000.000 1000.00
 1
 4.14394211E+00 5.59738818E-03-1.99794019E-06 3.16179193E-10-1.85614483E-
 14 2
 -1.72459887E+04 5.07778617E+00 4.68825921E+00-4.14871834E-03 2.55066010E-
 05 3
 -2.84473900E-08 1.04422559E-11-1.69867041E+04 4.28426480E+00-
 1.55992356E+04 4
 HOCH2O2H 9/ 1/12 C 1H 40 3 0G 300.000 5000.000
 1398.000 21
 1.24531886E+01 7.18221110E-03-2.47029548E-06 3.85611737E-10-2.24774193E-
 14 2
 -4.24862928E+04-3.58745197E+01 5.35189713E-01 3.73266553E-02-3.15299511E-
 05 3
 1.30352583E-08-2.11473264E-12-3.86609415E+04 2.71776082E+01
 4
 HOCH2O2 9/ 1/12 C 1H 30 3 0G 300.000 5000.000
 1377.000 21
 1.16406115E+01 5.72826040E-03-2.05362036E-06 3.29070695E-10-1.95188360E-
 14 2
 -2.53505769E+04-3.07332064E+01 2.82068616E+00 2.47857094E-02-1.66186399E-
 05 3
 4.79633095E-09-4.28087766E-13-2.22077036E+04 1.70599803E+01
 4
 OCH2O2H 11/21/14 THERMC 1H 30 3 0G 300.000 5000.000
 1384.000 21
 1.00715842E+01 8.14479426E-03-3.09415160E-06 5.10172792E-10-3.07179360E-
 14 2
 -1.43614053E+04-2.40065056E+01 3.77931486E+00 2.10896488E-02-1.29621750E-
 05 3
 3.84535112E-09-4.56757825E-13-1.19570349E+04 1.04826091E+01
 4
 HOCH2O 2/16/99 THERMC 1H 30 2 0G 300.000 5000.000
 1452.000 11
 6.39521515E+00 7.43673043E-03-2.50422354E-06 3.84879712E-10-2.21778689E-
 14 2
 -2.41108840E+04-6.63865583E+00 4.11183145E+00 7.53850697E-03 3.77337370E-
 06 3
 -5.38746005E-09 1.45615887E-12-2.28023001E+04 7.46807254E+00
 4
 CH3OH T06/02C 1H 4 O 1 0 G 200.000 6000.00 1000.00
 1
 3.52726795E+00 1.03178783E-02-3.62892944E-06 5.77448016E-10-3.42182632E-
 14 2
 -2.60028834E+04 5.16758693E+00 5.65851051E+00-1.62983419E-02 6.91938156E-
 05 3
 -7.58372926E-08 2.80427550E-11-2.56119736E+04-8.97330508E-01-
 2.41746056E+04 4
 CH2OH IU2/03C 1 H 3 O 1 0 G 200.000 6000.00
 1000.00 1
 5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-
 14 2
 -4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-
 05 3

-3.64869060E-08 1.47907450E-11-3.50072890E+03 3.30913500E+00-
 2.04462770E+03 4
 CH3O IU1/03C 1 H 3 O 1 0 G 200.000 6000.00 1000.00
 1
 4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-
 14 2
 3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-
 05 3
 -4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00
 2.52571660E+03 4
 CH3O2H A 7/05C 1 H 4 O 2 0 G 200.000 6000.00 1000.00
 1
 7.76538058E+00 8.61499712E-03-2.98006935E-06 4.68638071E-10-2.75339255E-
 14 2
 -1.82979984E+04-1.43992663E+01 2.90540897E+00 1.74994735E-02 5.28243630E-
 06 3
 -2.52827275E-08 1.34368212E-11-1.68894632E+04 1.13741987E+01-
 1.52423685E+04 4
 CH3O2 H 3C 1O 2 0G 300.000 5000.000
 1374.000 11!RE-FIT 0309
 6.47970487E+00 7.44401080E-03-2.52348555E-06 3.89577296E-10-2.25182399E-
 14 2
 -1.56285441E+03-8.19477074E+00 1.97339205E+00 1.53542340E-02-6.37314891E-
 06 3
 3.19930565E-10 2.82193915E-13 2.54278835E+02 1.69194215E+01
 4
 CH2O2H 9/ 1/12 C 1H 3O 2 0G 300.000 5000.000
 1410.000 21
 9.24697852E+00 4.60845541E-03-1.53501472E-06 2.34434830E-10-1.34573106E-
 14 2
 4.11529953E+03-2.11503248E+01 2.88976454E+00 2.09465776E-02-1.75190772E-
 05 3
 7.27819787E-09-1.18912344E-12 6.12390620E+03 1.23802076E+01
 4
 CH4 G 8/99C 1 H 4 0 0 G 200.000 6000.00 1000.00
 1
 1.65326226E+00 1.00263099E-02-3.31661238E-06 5.36483138E-10-3.14696758E-
 14 2
 -1.00095936E+04 9.90506283E+00 5.14911468E+00-1.36622009E-02 4.91453921E-
 05 3
 -4.84246767E-08 1.66603441E-11-1.02465983E+04-4.63848842E+00-
 8.97226656E+03 4
 CH3 IU0702C 1 H 3 0 0 G 200.000 6000.00 1000.00
 1
 0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-
 13 2
 0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-
 05 3
 -0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01
 0.17643935E+05 4
 CH2 IU3/03C 1 H 2 0 0 G 200.000 6000.00 1000.00
 1
 3.14631886E+00 3.03671259E-03-9.96474439E-07 1.50483580E-10-8.57335515E-
 15 2
 4.60412605E+04 4.72341711E+00 3.71757846E+00 1.27391260E-03 2.17347251E-
 06 3
 -3.48858500E-09 1.65208866E-12 4.58723866E+04 1.75297945E+00
 4.70504920E+04 4

CH2(S) IU6/03C 1 H 2 0 0 G 200.000 6000.00 1000.00
 1
 3.13501686E+00 2.89593926E-03-8.16668090E-07 1.13572697E-10-6.36262835E-
 15 2
 5.05040504E+04 4.06030621E+00 4.19331325E+00-2.33105184E-03 8.15676451E-
 06 3
 -6.62985981E-09 1.93233199E-12 5.03662246E+04-7.46734310E-01
 5.15727280E+04 4
 CH IU3/03C 1 H 1 0 0 G 200.000 6000.00 1000.00
 1
 0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-
 14 2
 0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-
 05 3
 0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01
 0.71658188E+05 4
 CH* 073003C 1H 1 G 0300.00 5000.00 1000.00
 1
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-
 13 2
 0.10419559E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-
 04 3
 0.05733890E-07-0.01955533E-10 0.10393714E+06 0.03331587E+02
 4
 C L 7/88C 1 0 0 OG 200.000 6000.00 1000.00
 1
 0.26055830E+01-0.19593434E-03 0.10673722E-06-0.16423940E-10 0.81870580E-
 15 2
 0.85411742E+05 0.41923868E+01 0.25542395E+01-0.32153772E-03 0.73379223E-
 06 3
 -0.73223487E-09 0.26652144E-12 0.85442681E+05 0.45313085E+01
 0.86195097E+05 4
 C2H6 G 8/88C 2H 6 0 OG 200.000 6000.00 1000.00
 1
 4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-
 14 2
 -1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-
 05 3
 -7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00-
 1.00849652E+04 4
 C2H5 8/ 4/ 4 THERMC 2H 5 0 OG 300.000 5000.000
 1387.000 11
 5.88784390E+00 1.03076793E-02-3.46844396E-06 5.32499257E-10-3.06512651E-
 14 2
 1.15065499E+04-8.49651771E+00 1.32730217E+00 1.76656753E-02-6.14926558E-
 06 3
 -3.01143466E-10 4.38617775E-13 1.34284028E+04 1.71789216E+01
 4
 C2H4 G 1/00C 2 H 4 0 0 G 200.000 6000.00 1000.00
 1
 3.99182724E+00 1.04833908E-02-3.71721342E-06 5.94628366E-10-3.53630386E-
 14 2
 4.26865851E+03-2.69081762E-01 3.95920063E+00-7.57051373E-03 5.70989993E-
 05 3
 -6.91588352E-08 2.69884190E-11 5.08977598E+03 4.09730213E+00
 6.31426266E+03 4
 C2H3 ATCT/AC 2 H 3 0 0 G 200.000 6000.00 1000.00
 1

4.15026763E+00 7.54021341E-03-2.62997847E-06 4.15974048E-10-2.45407509E-
 14 2
 3.38566380E+04 1.72812235E+00 3.36377642E+00 2.65765722E-04 2.79620704E-
 05 3
 -3.72986942E-08 1.51590176E-11 3.44749589E+04 7.91510092E+00
 3.56701718E+04 4
 C2H2 G 1/91C 2 H 2 0 0 G 200.000 6000.00 1000.00
 1
 4.65878489E+00 4.88396667E-03-1.60828888E-06 2.46974544E-10-1.38605959E-
 14 2
 2.57594042E+04-3.99838194E+00 8.08679682E-01 2.33615762E-02-3.55172234E-
 05 3
 2.80152958E-08-8.50075165E-12 2.64289808E+04 1.39396761E+01
 2.74459950E+04 4
 C2H T 5/10C 2 H 1 0 0 G 200.000 6000.00 1000.00
 1
 3.66270248E+00 3.82492252E-03-1.36632500E-06 2.13455040E-10-1.23216848E-
 14 2
 6.71683790E+04 3.92205792E+00 2.89867676E+00 1.32988489E-02-2.80733327E-
 05 3
 2.89484755E-08-1.07502351E-11 6.70616050E+04 6.18547632E+00
 6.83210436E+04 4
 CH3CHO L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00
 1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-
 13 2
 -0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-
 04 3
 -0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-
 0.19987949E+05 4
 CH3CO IU2/03C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
 1
 0.53137165E+01 0.91737793E-02-0.33220386E-05 0.53947456E-09-0.32452368E-
 13 2
 -0.36450414E+04-0.16757558E+01 0.40358705E+01 0.87729487E-03 0.30710010E-
 04 3
 -0.39247565E-07 0.15296869E-10-0.26820738E+04 0.78617682E+01-
 0.12388039E+04 4
 CH2CHO T03/10C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
 1
 6.53928338E+00 7.80238629E-03-2.76413612E-06 4.42098906E-10-2.62954290E-
 14 2
 -1.18858659E+03-8.72091393E+00 2.79502600E+00 1.01099472E-02 1.61750645E-
 05 3
 -3.10303145E-08 1.39436139E-11 1.62944975E+02 1.23646657E+01
 1.53380440E+03 4
 CH2CO H 2C 2O 1 0G 300.000 5000.000
 1391.000 01
 6.60179400E+00 5.23168519E-03-1.79376283E-06 2.82183642E-10-1.65610107E-
 14 2
 -8.61085819E+03-1.13932316E+01 1.65982341E+00 1.74426787E-02-1.35629541E-
 05 3
 5.53065784E-09-9.24027432E-13-6.95849922E+03 1.49168757E+01
 4
 HCCO T 4/09H 1 C 2 O 1 0 G 200.000 6000.00 1000.00
 1
 5.91479333E+00 3.71408730E-03-1.30137010E-06 2.06473345E-10-1.21476759E-
 14 2

1.93596301E+04-5.50567269E+00 1.87607969E+00 2.21205418E-02-3.58869325E-
 05 3
 3.05402541E-08-1.01281069E-11 2.01633840E+04 1.36968290E+01
 2.14444387E+04 4
 HCCOH T12/09C 2 H 2 O 1 0 G 200.000 6000.00 1000.00
 1
 6.37509678E+00 5.49429011E-03-1.88136576E-06 2.93803536E-10-1.71771901E-
 14 2
 8.93277676E+03-8.24498007E+00 2.05541154E+00 2.52003372E-02-3.80821654E-
 05 3
 3.09890632E-08-9.89799902E-12 9.76872113E+03 1.22271534E+01
 1.12217316E+04 4
 CH3CO3H 6/26/95 THERMC 2H 40 3 0G 300.000 5000.000
 1391.000 31
 1.25060485E+01 9.47789695E-03-3.30402246E-06 5.19630793E-10-3.04233568E-
 14 2
 -4.59856703E+04-3.79195947E+01 2.24135876E+00 3.37963514E-02-2.53887482E-
 05 3
 9.67583587E-09-1.49266157E-12-4.24677831E+04 1.70668133E+01
 4
 CH3CO3 4/ 3/ 0 THERMC 2H 30 3 0G 300.000 5000.000
 1391.000 21
 1.12522498E+01 8.33652672E-03-2.89014530E-06 4.52781734E-10-2.64354456E-
 14 2
 -2.60238584E+04-2.96370457E+01 3.60373432E+00 2.70080341E-02-2.08293438E-
 05 3
 8.50541104E-09-1.43846110E-12-2.34205171E+04 1.12014914E+01
 4
 CH3CO2 2/14/95 THERMC 2H 30 2 0G 300.000 5000.000
 1395.000 11
 8.54059736E+00 8.32951214E-03-2.84722010E-06 4.41927196E-10-2.56373394E-
 14 2
 -2.97290678E+04-2.03883545E+01 1.37440768E+00 2.49115604E-02-1.74308894E-
 05 3
 6.24799508E-09-9.09516835E-13-2.72330150E+04 1.81405454E+01
 4
 C2H5OH L 8/88C 2 H 6 O 1 0 G 200.000 6000.00 1000.00
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 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-
 13 2
 -0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-
 04 3
 -0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-
 0.28257829E+05 4
 PC2H4OH T12/01C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 7.02824536E+00 1.20037746E-02-4.21306455E-06 6.69471213E-10-3.96371893E-
 14 2
 -5.92493321E+03-9.40355948E+00 4.47893092E+00 7.59782301E-03 2.81794908E-
 05 3
 -4.26953487E-08 1.78878934E-11-4.71446256E+03 6.38921206E+00-
 2.86833500E+03 4
 SC2H4OH T10/04C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-4.03713238E-
 14 2
 -9.37900432E+03-6.05106112E+00 4.22283250E+00 5.12174798E-03 3.48386522E-
 05 3

-4.91943637E-08 2.01183723E-11-8.20503939E+03 8.01675700E+00-
6.49827831E+03 4
C2H5O IU2/03C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
1
0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-
13 2
-0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-
04 3
-0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-
0.16357022E+04 4
O2C2H4OH 9/ 1/12 THERMC 2H 50 3 0G 300.000 5000.000
1506.000 41
1.27503881E+01 1.11514325E-02-3.83473891E-06 5.98155829E-10-3.48372108E-
14 2
-2.52770876E+04-3.54317608E+01 7.04009800E+00 1.59564166E-02 2.21097416E-
06 3
-7.05197355E-09 2.08266026E-12-2.24524432E+04-1.75361758E+00
4
C2H5O2H 9/ 1/12 C 2H 60 2 0G 300.000 5000.000
1390.000 31
1.04823538E+01 1.34779879E-02-4.62179078E-06 7.18618519E-10-4.17307436E-
14 2
-2.46578171E+04-2.84294243E+01 1.83755328E+00 3.38053586E-02-2.37548140E-
05 3
9.31974865E-09-1.58003428E-12-2.15814086E+04 1.80977584E+01
4
C2H5O2 9/ 1/12 C 2H 50 2 0G 300.000 5000.000
1389.000 21
9.50282570E+00 1.20429839E-02-4.09491581E-06 6.33049241E-10-3.66133788E-
14 2
-7.37069391E+03-2.21717130E+01 3.90351912E+00 2.22599212E-02-1.01610079E-
05 3
1.71709751E-09 1.88166738E-14-5.09654081E+03 8.98722750E+00
4
C2H4O2H 9/ 1/12 C 2H 50 2 0G 300.000 5000.000
1389.000 31
1.00590614E+01 1.13378955E-02-3.89403387E-06 6.06090687E-10-3.52212353E-
14 2
4.24048653E+02-2.32086536E+01 2.75788364E+00 2.88271987E-02-2.08302264E-
05 3
8.47401397E-09-1.48617610E-12 3.00153893E+03 1.59921711E+01
4
C2H4O1-2 L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00
1
0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-
13 2
-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-
04 3
-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-
0.63304657E+04 4
C2H3O1-2 A 1/05C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
1
5.60158035E+00 9.17613962E-03-3.28028902E-06 5.27903888E-10-3.15362241E-
14 2
1.71446252E+04-5.47228512E+00 3.58349017E+00-6.02275805E-03 6.32426867E-
05 3
-8.18540707E-08 3.30444505E-11 1.85681353E+04 9.59725926E+00
1.97814471E+04 4

CH3COCH3 2/14/13 THERMC 3H 60 1 0G 300.000 5000.000
 1381.000 21
 9.68478208E+00 1.45488533E-02-4.98681534E-06 7.75343101E-10-4.50297606E-14 2
 -3.10899721E+04-2.68395746E+01 1.14767529E+00 3.00731373E-02-1.37643759E-05 3
 1.89028808E-09 2.02896771E-13-2.76607074E+04 2.06153026E+01
 4
 CH3COCH2 2/14/13 THERMC 3H 50 1 0G 300.000 5000.000
 1387.000 21
 1.09524298E+01 1.11458668E-02-3.86262877E-06 6.05088857E-10-3.53293362E-14 2
 -9.60833727E+03-3.15622776E+01 1.13381826E+00 3.25095045E-02-2.10424651E-05 3
 6.64421151E-09-8.12618901E-13-6.04868361E+03 2.17158655E+01
 4
 CH3COCH2O2 2/14/13 THERMC 3H 50 3 0G 300.000 5000.000
 1397.000 31
 1.65756401E+01 1.06465489E-02-3.61368681E-06 5.59053564E-10-3.23832271E-14 2
 -2.42541401E+04-5.45304899E+01 1.19378141E+00 4.98027161E-02-4.17999508E-05 3
 1.74527607E-08-2.88198761E-12-1.93244224E+04 2.67877493E+01
 4
 CH2COCH2O2H THERMC 3H 50 3 0G 300.000 5000.000
 1395.000 41
 1.83434297E+01 9.47172521E-03-3.36699101E-06 5.36484229E-10-3.16966408E-14 2
 -1.99138281E+04-6.35875102E+01-9.41174287E-01 6.41925461E-02-6.40174562E-05 3
 3.11887343E-08-5.90316242E-12-1.41896095E+04 3.65452260E+01
 4
 CH3COCH2O 2/ 8/13 THERMC 3H 50 2 0G 300.000 5000.000
 2002.000 21
 9.84061707E+00 1.59181106E-02-5.85164644E-06 9.56160073E-10-5.75477263E-14 2
 -2.11214823E+04-2.12330791E+01 5.85960137E+00 1.78954926E-02 7.41506398E-07 3
 -5.40032753E-09 1.47393197E-12-1.90714739E+04 2.70987883E+00
 4
 O(CH2)2CO H 4C 3O 2 G 298.150 2000.000 1000.00
 1
 3.86689108E+00 2.61757926E-02-1.43284134E-05 3.76562939E-09-3.82007471E-13 2
 -2.46961120E+04 4.09873884E+00-1.02159595E+00 3.96862783E-02-2.55289481E-05 3
 5.18919007E-09 7.72967977E-13-2.34162415E+04 2.91937286E+01
 4
 C2H3OCH2 H 5C 3O 1 G 298.0 6000.0
 1000.0 1
 1.00397568E+01 1.18952742E-02-4.13512716E-06 6.51590471E-10-3.83196617E-14 2
 7.27301530E+03-2.57171542E+01-1.44860882E+00 5.42514911E-02-7.45556749E-05 3
 6.03597706E-08-2.01938036E-11 1.01608402E+04 3.16318657E+01
 4
 C2H3CHO KPS12 C 3H 4O 1 0G 300.000 5000.000
 1398.000 01

9.99155394E+00 9.82348001E-03-3.31203088E-06 5.09524422E-10-2.93821890E-
 14 2
 -1.25303509E+04-2.85168883E+01 7.33844455E-01 3.17482671E-02-2.29599468E-
 05 3
 8.42104232E-09-1.23613478E-12-9.38473548E+03 2.10308851E+01
 4
 C2H3CO KPS12 C 3H 30 1 0G 300.000 5000.000
 1395.000 01
 8.86032735E+00 8.48985205E-03-2.90350080E-06 4.50763986E-10-2.61524281E-
 14 2
 7.73489171E+03-2.06978792E+01 1.65335195E+00 2.57402596E-02-1.89009911E-
 05 3
 7.29174972E-09-1.16083226E-12 1.02020654E+04 1.78705872E+01
 4
 C3H5O KPS12 C 3H 50 1 0G 300.000 5000.000
 1402.000 01
 1.02638186E+01 1.17609932E-02-3.89837957E-06 5.92650815E-10-3.38867417E-
 14 2
 7.25938472E+03-2.75108651E+01 8.24068673E-01 3.46749909E-02-2.51786795E-
 05 3
 9.56781953E-09-1.48085302E-12 1.04203725E+04 2.28283070E+01
 4
 C2H5CHO T05/10C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
 1
 7.44085690E+00 1.77301764E-02-6.34081568E-06 1.02040803E-09-6.09461714E-
 14 2
 -2.60055814E+04-1.44195446E+01 4.24529681E+00 6.68296706E-03 4.93337933E-
 05 3
 -6.71986124E-08 2.67262347E-11-2.41473007E+04 6.90738560E+00-
 2.22688471E+04 4
 C2H5CO A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 6.52325448E+00 1.54211952E-02-5.50898157E-06 8.85889862E-10-5.28846399E-
 14 2
 -7.19631634E+03-5.19862218E+00 6.25722402E+00-9.17612184E-03 7.61190493E-
 05 3
 -9.05514997E-08 3.46198215E-11-5.91616484E+03 2.23330599E+00-
 3.94851891E+03 4
 CH2CH2CHO 8/10/ 4 THERMC 3H 50 1 0G 300.000 5000.000
 1363.000 21
 9.96855598E+00 1.61917946E-02-6.64161740E-06 1.15444520E-09-7.21981790E-
 14 2
 -4.16450354E+03-2.73971573E+01 8.36272659E+00-3.90712606E-03 3.59751257E-
 05 3
 -2.69209237E-08 5.98920261E-12-7.55243244E+02-9.53140102E+00
 4
 CH3CHCHO 8/10/ 4 THERMC 3H 50 1 0G 300.000 5000.000
 1253.000 21
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 14 2
 -8.34456062E+03-2.17652483E+01-2.72811212E+00 3.80354483E-02-1.96782132E-
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 4
 CH3OCH3 2/11/14 THERMC 2H 60 1 0G 300.000 5000.000
 1999.000 21
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 14 2

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 06 3
 -1.62279885E-09 6.84330155E-13-2.35494445E+04 1.45029944E+01
 4
 CH3OCH2 2/11/14 THERMC 2H 50 1 0G 300.000 5000.000
 1395.000 11
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 14 2
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 05 3
 3.37160213E-09-4.15077249E-13-1.37208255E+03 1.87548958E+01
 4
 CH3OCH2O2 2/12/14 THERMC 2H 50 3 0G 300.000 5000.000
 1441.000 21
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 05 3
 5.76033887E-09-6.16081571E-13-2.04433218E+04 1.39429608E+01
 4
 CH2OCH2O2H 2/12/14 THERMC 2H 50 3 0G 300.000 5000.000
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 14 2
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 05 3
 2.18379311E-08-4.11295947E-12-1.46498100E+04 2.98253164E+01
 4
 CH3OCH2O2H 2/12/14 THERMC 2H 60 3 0G 300.000 5000.000
 1404.000 31
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 14 2
 -4.06745921E+04-3.78047802E+01 1.05786981E+00 4.36787095E-02-3.46383899E-
 05 3
 1.44808830E-08-2.46100643E-12-3.68851076E+04 2.43391936E+01
 4
 CH3OCH2O 5/15/14 THERMC 2H 50 2 0G 300.000 5000.000
 1523.000 31
 9.81288609E+00 1.21313106E-02-4.30285768E-06 6.84443177E-10-4.03862658E-
 14 2
 -2.50760742E+04-2.51866352E+01 5.63414373E+00 8.92830283E-03 1.37225633E-
 05 3
 -1.40497059E-08 3.54625624E-12-2.22825214E+04 1.93588846E+00
 4
 O2CH2OCH2O2H 2/12/14 ERM C 2H 50 5 0G 300.000 5000.000
 1433.000 31
 1.77378326E+01 1.13589899E-02-3.67382539E-06 5.49255712E-10-3.10405899E-
 14 2
 -3.82903058E+04-5.66609932E+01 2.39977678E+00 5.39881943E-02-4.87969524E-
 05 3
 2.19792134E-08-3.86106979E-12-3.37824638E+04 2.30683371E+01
 4
 HO2CH2OCHO 2/12/14 THERMC 2H 40 4 0G 300.000 5000.000
 1386.000 31
 1.57136128E+01 9.64430166E-03-3.44136025E-06 5.49722196E-10-3.25360322E-
 14 2
 -6.29409094E+04-5.29505242E+01 1.21909586E+00 4.28858235E-02-3.17634222E-
 05 3

1.11542676E-08-1.49753153E-12-5.79287926E+04 2.49759193E+01
 4
 OCH2OCHO 5/29/14 THERMC 2H 30 3 0G 300.000 5000.000
 1523.000 21
 1.24013200E+01 7.83738243E-03-2.82992688E-06 4.55558739E-10-2.71061389E-
 14 2
 -4.68453470E+04-3.78084549E+01 1.89539692E+00 2.74118545E-02-1.36476090E-
 05 3
 1.26325603E-09 5.17970476E-13-4.27879440E+04 2.02333278E+01
 4
 HOCH2OCO 5/29/14 THERMC 2H 30 3 0G 300.000 5000.000
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 1.11498410E+01 9.34736520E-03-3.35541548E-06 5.38037115E-10-3.19260183E-
 14 2
 -4.75012119E+04-2.95983867E+01 5.95255071E+00 8.42196282E-03 1.36741678E-
 05 3
 -1.46786275E-08 3.84143533E-12-4.44470269E+04 2.85657217E+00
 4
 CH3OCHO T 6/08C 2 H 4 O 2 0 G 200.000 6000.00 1000.00
 1
 6.33360880E+00 1.34851485E-02-4.84305805E-06 7.81719241E-10-4.67917447E-
 14 2
 -4.68316521E+04-6.91542601E+00 5.96757028E+00-9.38085425E-03 7.07648417E-
 05 3
 -8.29932227E-08 3.13522917E-11-4.55713267E+04 7.50341113E-01-
 4.37330508E+04 4
 CH3OCO 5/ 8/ 3 THERMC 2H 30 2 0G 300.000 5000.000
 1601.000 21
 9.73659803E+00 7.42432713E-03-2.65641779E-06 4.25031143E-10-2.51824924E-
 14 2
 -2.36015721E+04-2.36353471E+01 4.16215406E+00 1.38037511E-02-3.08486109E-
 07 3
 -4.56430814E-09 1.46909632E-12-2.10130301E+04 8.64301044E+00
 4
 CH2OCHO 4/15/ 8 THERMC 2H 30 2 0G 300.000 5000.000
 1442.000 21
 1.00960096E+01 7.19887066E-03-2.59813465E-06 4.18110812E-10-2.48723387E-
 14 2
 -2.36389018E+04-2.71144175E+01 2.31031671E+00 1.80474065E-02-2.71519637E-
 06 3
 -4.60918579E-09 1.70037078E-12-2.02910878E+04 1.71549722E+01
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 HE G 5/97HE 1 0 0 0 G 200.000 6000.00 1000.00
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 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01
 0.00000000E+00 4
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 -1.62754066E+04-1.31943379E+01 4.21093013E+00 1.70886504E-03 7.06530164E-
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 1.25900384E+04 4

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 1.21859256E+04 4
 IC3H7 A 5/05C 3 H 7 0 0 G 200.000 6000.00 1000.00
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 5.30597255E+00 1.89854588E-02-6.74315384E-06 1.07993730E-09-6.42785036E-
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 7.78748910E+03-2.23233935E+00 5.47421257E+00-8.42536682E-03 8.04607759E-
 05 3
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 1.08473019E+04 4
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 14 2
 -7.41715057E+02-8.43825992E+00 3.83464468E+00 3.29078952E-03 5.05228001E-
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 2.40543339E+03 4
 C3H5-A PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
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 0.65007877E+01 0.14324731E-01-0.56781632E-05 0.11080801E-08-0.90363887E-
 13 2
 0.17482449E+05-0.11243050E+02 0.13631835E+01 0.19813821E-01 0.12497060E-
 04 3
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 4
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 1
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 13 2
 0.27843027E+05-0.33527184E+01 0.17329209E+01 0.22394620E-01-0.51490611E-
 05 3
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 4
 C3H5-S PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
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 13 2
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 04 3
 -0.23035678E-08 0.27715488E-11 0.30916867E+05 0.19989269E+02
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 13 2
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 04 3
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 0.22962267E+05 4
 C3H4-P T 2/90H 4 C 3 0 0 G 200.000 6000.00 1000.00
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 05 3
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 0.22302059E+05 4
 C3H3 T 7/11C 3 H 3 0 0 G 200.000 6000.00
 1000.000 1
 7.14221719E+00 7.61902211E-03-2.67460030E-06 4.24914904E-10-2.51475443E-
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 05 3
 3.76310220E-08-1.18541128E-11 4.07679941E+04 1.52058598E+01
 4.22762135E+04 4
 C3H3O 2/17/14 CZHOUH 3C 3O 1 G 298.150 2000.000 1000.00
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 4.19355696E+00 1.95625103E-02-1.22336450E-05 3.90615061E-09-5.08539231E-
 13 2
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 05 3
 2.40255750E-08-6.10883631E-12 3.20427921E+04 2.04717253E+01
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 C3H3O2H 1/31/13 C 3H 4O 2 OG 300.000 5000.000
 1385.000 31
 1.38152174E+01 8.62174763E-03-3.06710006E-06 4.88874247E-10-2.88888385E-
 14 2
 6.29182941E+03-4.39151257E+01 1.09787313E+00 4.22717882E-02-3.83969355E-
 05 3
 1.77405069E-08-3.27674312E-12 1.03592314E+04 2.30651783E+01
 4
 C2HCHO 1/31/13 C 3H 2O 1 OG 300.000 5000.000
 2012.000 11
 7.99952054E+00 7.07825497E-03-2.63086819E-06 4.33073185E-10-2.62003284E-
 14 2
 8.71863156E+03-1.57226237E+01 4.20776611E+00 1.34382727E-02-5.15442099E-
 06 3
 -2.24570818E-11 2.74111284E-13 1.02117375E+04 5.43871873E+00
 4
 C3H2 T12/00C 3 H 2 0 0 G 200.000 6000.00 1000.00
 1
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 14 2
 7.57571184E+04-9.72894405E+00 2.43417332E+00 1.73013063E-02-1.18294047E-
 05 3
 1.02756396E-09 1.62626314E-12 7.69074892E+04 1.21012230E+01
 7.83005132E+04 4
 C3H2(S) OC 3H 2 0 OG 200.000 5000.000 900.00
 0 1
 0.77642570E+01 0.47112774E-02-0.16170637E-05 0.25472406E-09-0.15038572E-
 13 2
 0.66849672E+05-0.15098549E+02 0.52976482E+01 0.16987466E-01-0.24266517E-
 04 3
 0.18653681E-07-0.55763001E-11 0.67240466E+05-0.37540041E+01
 4
 C3H2C OC 3H 2 0 OG 200.000 5000.000 1500.00
 0 1
 0.65632680E+01 0.52363256E-02-0.17544830E-05 0.26866106E-09-0.15428509E-
 13 2

0.56514618E+05-0.12000607E+02 0.11295888E+01 0.17287401E-01-0.11366823E-
 04 3
 0.34569296E-08-0.36615951E-12 0.58419080E+05 0.17331448E+02
 4
 H2CCC(S) OC 3H 2 0 OG 200.000 5000.000 1500.00
 0 1
 0.64888762E+01 0.53112789E-02-0.17809490E-05 0.27252642E-09-0.15619590E-
 13 2
 0.63661864E+05-0.10064283E+02 0.37229726E+01 0.92589854E-02-0.23006191E-
 05 3
 -0.10200808E-08 0.45374357E-12 0.64877289E+05 0.56865936E+01
 4
 C3H6OOH1-3 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1401.000 41
 1.39130757E+01 1.40218463E-02-4.55921149E-06 6.84182417E-10-3.87696213E-
 14 2
 -3.65650518E+03-4.21532559E+01 1.74271107E+00 4.53733504E-02-3.57580373E-
 05 3
 1.48540053E-08-2.49981756E-12 2.32580844E+02 2.20973041E+01
 4
 C3H6OOH1-2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1387.000 41
 1.38088686E+01 1.43845650E-02-4.74440961E-06 7.19308280E-10-4.10654123E-
 14 2
 -5.14352831E+03-4.20210765E+01 2.83631132E+00 3.88229894E-02-2.47944364E-
 05 3
 7.85644898E-09-9.58634300E-13-1.26002528E+03 1.72549973E+01
 4
 C3H6OOH2-1 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1393.000 41
 1.36645362E+01 1.54329764E-02-5.29285952E-06 8.23001262E-10-4.77931121E-
 14 2
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 1387.000 41
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 14 2
 -8.96332407E+03-3.66195515E+01 5.31236076E+00 3.16261247E-02-1.81191476E-
 05 3
 5.81572618E-09-8.62108993E-13-6.02627337E+03 4.62683594E+00
 4
 C3H6OOH1-3O2 9/ 1/12 C 3H 7O 4 OG 300.000 5000.000
 1416.000 51
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 -2.26256376E+04-5.93719393E+01 5.56933350E+00 4.68523421E-02-3.58917784E-
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 1.43314525E-08-2.29776083E-12-1.86065694E+04 7.18655005E+00
 4
 C3H6OOH1-2O2 9/ 1/12 C 3H 7O 4 OG 300.000 5000.000
 1404.000 51
 1.91044980E+01 1.44076100E-02-4.72127814E-06 7.12631642E-10-4.05578490E-
 14 2
 -2.50270510E+04-6.63747978E+01 3.99085043E+00 5.31865338E-02-4.28597948E-
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1.77187019E-08-2.92768695E-12-2.02143526E+04 1.34150719E+01
 4
 C3H6OOH2-1O2 9/ 1/12 C 3H 7O 4 OG 300.000 5000.000
 1404.000 51
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 4
 NC3H7O T07/10C 3 H 7 O 1 0 G 200.000 6000.00 1000.00
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 05 3
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 4.26576768E+03 4
 IC3H7O 9/ 1/12 C 3H 7O 1 OG 300.000 5000.000
 1386.000 21
 1.14627518E+01 1.51011907E-02-5.07470532E-06 7.78736627E-10-4.48206286E-
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 05 3
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 4
 NC3H7O2H 9/ 1/12 C 3H 8O 2 OG 300.000 5000.000
 1394.000 41
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 1.30546796E-08-1.95621807E-12-2.43818102E+04 2.40611651E+01
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 NC3H7O2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
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 IC3H7O2H 9/ 1/12 C 3H 8O 2 OG 300.000 5000.000
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 4
 IC3H7O2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1395.000 31
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 14 2
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 05 3
 8.80154103E-09-1.31154059E-12-9.90211798E+03 1.03892668E+01
 4

C3H6O1-3 A11/04C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
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14 2
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-1.58629974E-07 6.20668783E-11-1.13243512E+04 4.73561224E+00-
9.75233898E+03 4
C3H6O1-2 A01/05C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
1
8.01491079E+00 1.73919953E-02-6.26027968E-06 1.01188256E-09-6.06239111E-
14 2
-1.51980838E+04-1.88279964E+01 3.42806676E+00 6.25176642E-03 6.13196311E-
05 3
-8.60387185E-08 3.51371393E-11-1.28446646E+04 1.04244994E+01-
1.11564001E+04 4
C3KET21 2/14/13 THERMC 3H 6O 3 0G 300.000 5000.000
1394.000 41
1.75768076E+01 1.20311704E-02-4.11633942E-06 6.40149366E-10-3.72127562E-
14 2
-4.15502347E+04-6.09097100E+01-8.74352903E-01 6.12501498E-02-5.51474542E-
05 3
2.48491014E-08-4.42613472E-12-3.58060819E+04 3.59306224E+01
4
C3H51-2,3OOH 8/26/3 THRMC 3H 7O 4 0G 300.000 5000.000
1386.000 61
2.12378169E+01 1.39519596E-02-4.94539222E-06 7.86381389E-10-4.63925564E-
14 2
-1.92864584E+04-7.69636561E+01 2.55619708E+00 6.13504487E-02-5.23205391E-
05 3
2.28208029E-08-4.02231508E-12-1.31353414E+04 2.21043799E+01
4
C3H52-1,3OOH 8/26/3 THRMC 3H 7O 4 0G 300.000 5000.000
1379.000 61
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14 2
-1.80085066E+04-7.22688262E+01 4.12253742E+00 5.19553611E-02-3.83733727E-
05 3
1.45851637E-08-2.29820536E-12-1.22759164E+04 1.48367359E+01
4
C3H6OH1-2 9/ 1/12 C 3H 7O 1 0G 300.000 5000.000
1395.000 31
1.00338281E+01 1.60227373E-02-5.41658448E-06 8.34191172E-10-4.81215988E-
14 2
-1.27912397E+04-2.39034395E+01 5.05207596E-01 3.63869988E-02-2.15530901E-
05 3
6.45584786E-09-7.71267046E-13-9.26980840E+03 2.79804349E+01
4
TQJC3H6OH C 3H 7O 3 0G 300.000 5000.000
1411.000 41
1.57530365E+01 1.56289438E-02-5.23690385E-06 8.01741456E-10-4.60590728E-
14 2
-3.24130576E+04-5.08911217E+01 2.29728737E+00 4.96725824E-02-3.84714645E-
05 3
1.56038090E-08-2.56748169E-12-2.80429510E+04 2.03767936E+01
4
TQC3H6OI C 3H 7O 3 0G 300.000 5000.000
1417.000 41

1.71497525E+01 1.47440875E-02-4.99973196E-06 7.71920259E-10-4.46175680E-
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 05 3
 9.92338649E-09-1.22338206E-12-1.84544341E+04 1.23546787E+01
 4
 QC3H5OHP C 3H 70 3 OG 300.000 5000.000
 1415.000 51
 1.65390643E+01 1.45962463E-02-4.89569717E-06 7.50190330E-10-4.31310565E-
 14 2
 -2.47102324E+04-5.34015731E+01 1.76951547E+00 5.23733147E-02-4.19658180E-
 05 3
 1.72471815E-08-2.83710014E-12-1.99859353E+04 2.46273265E+01
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 -2.63164910E+04-4.81509679E+01 5.58028765E+00 3.00649782E-02-6.38519910E-
 06 3
 -4.74322634E-09 1.89822226E-12-2.19537872E+04 8.64790031E+00
 4
 CCY(COC)OH C 3H 60 2 OG 300.000 5000.000
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 1.37176873E+01 1.33634818E-02-4.51490840E-06 6.95521032E-10-4.01451866E-
 14 2
 -4.07527954E+04-4.74449508E+01-7.68565795E-01 4.79603507E-02-3.53347028E-
 05 3
 1.27934873E-08-1.79555386E-12-3.59177637E+04 2.98848715E+01
 4
 IQJC3H6OH C 3H 70 3 OG 300.000 5000.000
 1408.000 41
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 14 2
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 05 3
 1.66120004E-08-2.78425352E-12-2.79317094E+04 2.33734165E+01
 4
 IQC3H6OT C 3H 70 3 OG 300.000 5000.000
 1406.000 41
 1.67044548E+01 1.52497437E-02-5.19996341E-06 8.05676289E-10-4.66785083E-
 14 2
 -2.29660389E+04-5.69717854E+01 2.97554636E+00 4.80962295E-02-3.51787999E-
 05 3
 1.32008460E-08-2.00208137E-12-1.83154710E+04 1.64182550E+01
 4
 IQC3H5OHPJ C 3H 70 3 OG 300.000 5000.000
 1409.000 51
 1.59552559E+01 1.50895186E-02-5.06382338E-06 7.76108726E-10-4.46235236E-
 14 2
 -2.45035338E+04-4.99018045E+01 1.35929059E+00 5.34300669E-02-4.41305751E-
 05 3
 1.89646022E-08-3.27838412E-12-1.98996889E+04 2.69126449E+01
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 1379.000 31
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 14 2

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 05 3
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 4
 CHOCH2OOH C 2H 40 3 0G 300.000 5000.000
 1391.000 31
 1.51554685E+01 7.57240000E-03-2.72693024E-06 4.38217189E-10-2.60434287E-
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 -3.41419680E+04-5.08149884E+01-1.32768631E+00 5.21618601E-02-4.97327645E-
 05 3
 2.31272366E-08-4.20787867E-12-2.90608844E+04 3.54965675E+01
 4
 CY(CCOC)OH C 3H 60 2 0G 300.000 5000.000
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 2.68222743E-08-4.79465381E-12-3.07734013E+04 5.39539327E+01
 4
 CHOCOHC3 C 3H 60 2 0G 300.000 5000.000
 1379.000 31
 1.36133542E+01 1.38716512E-02-4.87445259E-06 7.70639716E-10-4.52818606E-
 14 2
 -4.85836793E+04-4.37863752E+01 9.59562607E-01 4.04355781E-02-2.52333819E-
 05 3
 7.47748757E-09-8.33450351E-13-4.38727633E+04 2.52653125E+01
 4
 CY(COC)COH C 3H 60 2 0G 300.000 5000.000
 1427.000 21
 1.23650178E+01 1.37866121E-02-4.50198310E-06 6.77071535E-10-3.84092609E-
 14 2
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 05 3
 2.38463400E-08-4.27986682E-12-3.04628787E+04 4.23855523E+01
 4
 TQC3H5OHIO2 C 3H 70 5 0G 300.000 5000.000
 1387.000 61
 2.02916342E+01 1.92145529E-02-8.58823433E-06 1.62509037E-09-1.06225627E-
 13 2
 -4.85976512E+04-7.10879629E+01 2.11774097E+00 7.25997025E-02-6.81667819E-
 05 3
 3.13796075E-08-5.68565078E-12-4.35518506E+04 2.23586550E+01
 4
 TQC3H5OHIOQ-I C 3H 70 5 0G 300.000 5000.000
 1391.000 61
 2.28708932E+01 1.56658128E-02-6.48662482E-06 1.17068411E-09-7.44373426E-
 14 2
 -3.97155885E+04-8.61588096E+01 3.46235675E+00 6.98705440E-02-6.48577576E-
 05 3
 2.96626742E-08-5.34536953E-12-3.39681675E+04 1.47596723E+01
 4
 TQC3H5OHIOQ-P C 3H 70 5 0G 300.000 5000.000
 1478.000 71
 2.59345778E+01 6.66525395E-03-1.66651304E-07-4.20552574E-10 5.49726117E-
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 05 3

2.79222006E-08-4.68412156E-12-3.56101660E+04 2.27189955E+01
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 C2H3COHOOH C 3H 60 3 0G 300.000 5000.000
 1393.000 41
 1.69349460E+01 1.32757225E-02-5.30958950E-06 9.43268930E-10-5.97339692E-14 2
 -3.77990580E+04-5.97614008E+01 3.73734021E-01 5.84060291E-02-5.29627415E-05 3
 2.38734015E-08-4.26063052E-12-3.27577137E+04 2.67905679E+01
 4
 COHOHCY (COC) C 3H 60 4 0G 300.000 5000.000
 1394.000 41
 1.78808618E+01 1.47154928E-02-5.11766843E-06 8.03382779E-10-4.69696797E-14 2
 -5.19254526E+04-6.47302080E+01-3.16180219E+00 7.92240221E-02-8.28674521E-05 3
 4.32049848E-08-8.69506663E-12-4.59891154E+04 4.31128002E+01
 4
 OHCY (COCC) OOH C 3H 60 4 0G 300.000 5000.000
 1520.000 31
 1.88928431E+01 1.38516388E-02-4.73692460E-06 7.36282623E-10-4.27819063E-14 2
 -5.31875949E+04-7.05664934E+01-2.13807799E-01 5.79347134E-02-4.16882857E-05 3
 1.38590975E-08-1.65613593E-12-4.67090699E+04 3.18890641E+01
 4
 IQC3H5OHPJO2 C 3H 70 5 0G 300.000 5000.000
 1407.000 61
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 -4.36087438E+04-7.05205391E+01 2.83411409E+00 6.29377015E-02-5.35228290E-05 3
 2.33491916E-08-4.06934890E-12-3.80451295E+04 2.27789799E+01
 4
 IQC3H5OTQ-I C 3H 70 5 0G 300.000 5000.000
 1415.000 61
 2.17590493E+01 1.51627633E-02-5.16409734E-06 7.99713840E-10-4.63243290E-14 2
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 1.70399951E-08-2.61590876E-12-2.85442590E+04 1.23781282E+01
 4
 IQC3H5OHQ-SJ C 3H 70 5 0G 300.000 5000.000
 1430.000 71
 2.01633063E+01 1.57355922E-02-5.28426264E-06 8.10536228E-10-4.66373245E-14 2
 -3.70242993E+04-6.56524053E+01 3.75150220E+00 5.60926263E-02-4.26964877E-05 3
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 4
 CHOCOHC2OOH C 3H 60 4 0G 300.000 5000.000
 1384.000 51
 1.86816278E+01 1.39658539E-02-4.94259642E-06 7.85147166E-10-4.62881931E-14 2
 -5.97999375E+04-6.41155772E+01 1.90697565E+00 5.29537602E-02-3.95708722E-05 3
 1.48146113E-08-2.23976588E-12-5.39646718E+04 2.60308355E+01
 4

CHOCHO C 2H 20 2 OG 300.000 5000.000
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 4
 TQC3H5OHTO2 C 3H 70 5 OG 300.000 5000.000
 1387.000 61
 2.02916342E+01 1.92145529E-02-8.58823433E-06 1.62509037E-09-1.06225627E-13 2
 -4.85976512E+04-7.10879629E+01 2.11774097E+00 7.25997025E-02-6.81667819E-05 3
 3.13796075E-08-5.68565078E-12-4.35518506E+04 2.23586550E+01
 4
 OHCOCOOHCH3 C 3H 60 4 OG 300.000 5000.000
 1393.000 51
 2.01819586E+01 1.34325042E-02-4.81163867E-06 7.56987137E-10-4.37448189E-14 2
 -7.33623538E+04-7.56343874E+01-1.96293682E-01 6.45815031E-02-5.49196882E-05 3
 2.34355354E-08-4.01181684E-12-6.66388685E+04 3.25552353E+01
 4
 HOC3H6O2 9/ 1/12 C 3H 70 3 OG 300.000 5000.000
 1407.000 41
 1.56948113E+01 1.57703692E-02-5.30501726E-06 8.14307835E-10-4.68666193E-14 2
 -3.24540840E+04-5.06084117E+01 2.84960487E+00 4.77244552E-02-3.60392974E-05 3
 1.43479922E-08-2.33507634E-12-2.82106103E+04 1.76478537E+01
 4
 CH3CHCO 03/03/95 THERMC 3H 40 1 OG 300.000 5000.000 1400.00
 41
 1.00219123E+01 9.56966300E-03-3.26221644E-06 5.05231706E-10-2.92593257E-14 2
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 1.20499164E-08-2.18365931E-12-1.15276540E+04 1.71552068E+01
 4
 AC3H5OOH GOLDSMITH C 3H 60 2 OG 298.0 6000.0
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 -1.02184463E+04-3.36434791E+01 3.18124993E+00 4.35233041E-02-5.16277353E-05 3
 4.32011427E-08-1.57714983E-11-7.63521503E+03 1.21725683E+01
 4
 AC4H7OOH 6/17/13 THERMC 4H 80 2 OG 300.000 5000.000
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 1.32495013E-08-2.06619289E-12-8.87891782E+03 2.43857336E+01
 4
 C2H3OOH 4/18/ 8 THERMC 2H 40 2 OG 300.000 5000.000
 1397.000 21

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 7.07078402E-09-6.98493372E-13-1.68794837E+04 2.63198718E+01
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 PC4H9 9/ 1/12 C 4H 9 0 0G 300.000 5000.000
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 05 3
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 SC4H9 9/ 1/12 C 4H 9 0 0G 300.000 5000.000
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 3.45938210E-09-2.39235619E-14 6.17688777E+03 2.52737918E+01
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 C4H8-1 T05/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
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 7.86795262E+00 2.24448843E-02-8.07705438E-06 1.30179988E-09-7.77958472E-
 14 2
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 3.72842176E+00 4
 C4H8-2 T 5/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
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 05 3
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 1.34523863E+03 4
 C4H71-1 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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 8.15646382E+00 1.90308835E-02-6.73262214E-06 1.07333098E-09-6.36886441E-
 14 2
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 05 3
 -6.30299109E-08 2.59475110E-11 2.75256555E+04 8.57181248E+00
 2.95712937E+04 4
 C4H71-2 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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 14 2

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 05 3
 -5.72714455E-08 2.36641011E-11 2.58014506E+04 9.11906641E+00
 2.78022108E+04 4
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 14 2
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 05 3
 -8.97456502E-08 3.61716165E-11 1.43843217E+04 7.30313471E+00
 1.63702936E+04 4
 C4H71-4 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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 2.46070249E+04 4
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 2.69231159E+04 4
 C4H6 H6W/94C 4H 6 0 0G 300.000 3000.00 1000.00
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 12 2
 0.91338516E+04-0.23328171E+02 0.11284465E+00 0.34369022E-01-0.11107392E-
 04 3
 -0.92106660E-08 0.62065179E-11 0.11802270E+05 0.23089996E+02
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 PC4H9O2H 9/ 1/12 C 4H 100 2 0G 300.000 5000.000
 1410.000 51
 1.85422067E+01 1.95532704E-02-6.40903366E-06 9.67561826E-10-5.50744230E-
 14 2
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 4
 PC4H9O2 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1663.000 41
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 -1.51651087E+04-5.27319441E+01 2.16957521E+00 5.22744687E-02-3.32954958E-
 05 3
 1.03030945E-08-1.20770740E-12-1.07180659E+04 2.03541558E+01
 4
 SC4H9O2H 9/ 1/12 C 4H 100 2 0G 300.000 5000.000
 1395.000 51
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 14 2
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 05 3

2.00008685E-08-3.25194364E-12-2.91704448E+04 2.63739532E+01
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 SC4H9O2 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
 1408.000 41
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 14 2
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 05 3
 1.22899616E-08-1.68623273E-12-1.27229421E+04 1.62316995E+01
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 PC4H9O 8/ 9/ 4 THERMC 4H 90 1 OG 300.000 5000.000
 1403.000 31
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 05 3
 1.08145957E-08-1.29600044E-12-9.11644218E+03 3.09183423E+01
 4
 SC4H9O 8/ 9/ 4 THERMC 4H 90 1 OG 300.000 5000.000
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 05 3
 1.01023834E-08-1.11268025E-12-1.11109627E+04 2.88554742E+01
 4
 C4H7O 4/ 3/ 0 THERMC 4H 70 1 OG 300.000 5000.000
 1395.000 21
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 14 2
 -7.29342884E+02-5.52937859E+01-1.60619192E+00 5.58562682E-02-4.35595767E-
 05 3
 1.70589279E-08-2.65635180E-12 4.85090326E+03 3.47112559E+01
 4
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 1399.000 21
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 14 2
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 05 3
 1.66679793E-08-2.64714350E-12-1.53950880E+04 3.66425242E+01
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 1371.000 51
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 05 3
 1.01079922E-08-1.10262736E-12-1.52980680E+04 3.67400719E+01
 4
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 1361.000 51
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 3.65743744E-09 3.94863161E-13-2.30067422E+04 4.19349253E+01
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C4H8O2-3 1/22/95 THERMC 4H 80 1 0G 300.000 5000.000
 1384.000 51
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 2.24064364E-08-3.95416618E-12-1.71957196E+04 3.66920390E+01
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 PC4H8OH 2/12/ 9 THERMC 4H 90 1 0G 300.000 5000.000
 1503.000 41
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 3.03714993E-09 3.72027554E-13-1.18622440E+04 2.65515175E+01
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 SC4H8OH 2/12/ 9 THERMC 4H 90 1 0G 300.000 5000.000
 1392.000 41
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 1.80944672E-08-3.02843329E-12-1.28718032E+04 3.48383489E+01
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 1396.000 51
 1.74383247E+01 2.16778876E-02-7.37772628E-06 1.14128811E-09-6.60391451E-14 2
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 1.53891643E-08-2.51940787E-12-3.05246721E+04 2.09293355E+01
 4
 C4H8OH-2O2 6/26/95 THERMC 4H 90 3 0G 300.000 5000.000
 1399.000 51
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 C4H8OOH1-1 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
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 1.80356600E+01 1.76337160E-02-5.78764161E-06 8.74574816E-10-4.98150150E-14 2
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 2.88403536E+04 4
 C2H5COCH2 4/ 3/ 0 THERMC 4H 70 1 OG 300.000 5000.000
 1383.000 31
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 4
 CH3CHOOCH3 6/27/95 C 4H 70 3 0G 300.000 5000.000 1393.00
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 2.47924787E+04 4
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 C3H6CHO-1 9/27/95 THERMC 4H 70 1 0G 300.000 5000.000
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 4

C3H6CHO-2 11/15/95 THERMC 4H 70 1 0G 300.000 5000.000
 1682.000 31
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 C3H6CHO-3 11/15/95 THERMC 4H 70 1 0G 300.000 5000.000
 1387.000 31
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 8.70132567E-09-1.15287455E-12-6.91166610E+03 2.09381509E+01
 4
 C2H5CHCO 9/27/95 THERMC 4H 60 1 0G 300.000 5000.000 1400.00
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 6.61981524E+03 4
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 IC4H7 C 4H 7 0 0G 300.000 5000.000
 1384.000 11
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 IC4H7-I1 5/13/15 C 4H 7 0 0G 300.000 5000.000
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 05 3
 -2.04641931E-09 1.18879408E-12-1.45627247E+04 1.58606320E+01
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 IC3H7CHO 2/22/96 THERMC 4H 80 1 0G 300.000 5000.000
 1391.000 31
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 14 2
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 05 3
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 TC3H6CHO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
 1389.000 21
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 14 2
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 05 3
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 4
 IC3H6CHO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
 1390.000 31
 1.33102250E+01 1.62097959E-02-5.57575891E-06 8.69003718E-10-5.05554202E-
 14 2
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 05 3
 9.30319894E-09-1.20761563E-12-2.99677086E+03 2.68182130E+01
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 IC3H7CO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
 1390.000 31
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 14 2
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 05 3
 8.93548675E-09-1.11327422E-12-9.07755468E+03 2.61991461E+01
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 IC4H8OOH-IO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
 1367.000 61
 2.24664901E+01 2.09351287E-02-7.44324128E-06 1.18589255E-09-7.00546897E-
 14 2
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 05 3
 7.79536931E-09-6.21665008E-13-2.22782534E+04 1.52623111E+01
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IC4H8OOH-TO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
 1385.000 61
 2.32464612E+01 1.88384513E-02-6.40938087E-06 9.92649459E-10-5.75275879E-
 14 2
 -3.16533132E+04-8.88301710E+01 3.36413530E+00 6.93742776E-02-5.70416393E-
 05 3
 2.46040165E-08-4.32848680E-12-2.51137558E+04 1.65767339E+01
 4
 TC4H8OOH-IO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
 1385.000 61
 2.32464612E+01 1.88384513E-02-6.40938087E-06 9.92649459E-10-5.75275879E-
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 2.46040165E-08-4.32848680E-12-2.51137558E+04 1.65767339E+01
 4
 IC4KETII 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 IC4KETIT 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 4
 IC4H7OH C 4H 80 1 0G 300.000 5000.000
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 14 2
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 IC4H7OOCH3 C 5H 100 2 0G 300.000 5000.000
 1386.000 51
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 2.27496198E-08-4.11475065E-12-1.16767937E+04 2.44900544E+01
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 SC4H7OH-I L 2/00C 4H 80 1 0G 300.000 5000.000
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 14 2
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 SC4H7OH-IP C 4H 70 1 0G 300.000 5000.000
 1402.000 21

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 14 2
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 05 3
 2.49299933E-08-4.52282491E-12-6.95012413E+03 3.20768458E+01
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 IC4H6OH 8/19/95 THERMC 4H 70 1 OG 300.000 5000.000
 1390.000 31
 1.40310926E+01 1.55317541E-02-5.32754961E-06 8.28785902E-10-4.81545257E-
 14 2
 -7.69378228E+03-4.76555306E+01 8.63371227E-01 4.68711282E-02-3.43580339E-
 05 3
 1.33031052E-08-2.13914975E-12-3.14948305E+03 2.29075523E+01
 4
 IC3H5CHO C 4H 60 1 OG 300.000 5000.000
 1396.000 21
 1.33892118E+01 1.39115420E-02-4.75820958E-06 7.38736618E-10-4.28606559E-
 14 2
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 05 3
 1.39369607E-08-2.33791460E-12-1.56745978E+04 1.94458467E+01
 4
 IC3H4CHO-A C 4H 50 1 OG 300.000 5000.000
 1392.000 11
 1.41736959E+01 1.09161978E-02-3.69020878E-06 5.69228087E-10-3.29023246E-
 14 2
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 05 3
 1.48295287E-08-2.43809290E-12 2.44732544E+03 2.08541848E+01
 4
 IC3H5OCH2 6/ 2/14 CZHOUH 7C 40 1 G 298.150 2000.000 1000.00
 1
 6.64731727E+00 3.08190709E-02-1.73209320E-05 5.01099629E-09-6.00089387E-
 13 2
 1.70679921E+03-5.91214819E+00-2.14798958E+00 7.00225553E-02-8.21595440E-
 05 3
 5.22589946E-08-1.34176532E-11 3.26474773E+03 3.55145589E+01
 4
 IC3H5CO C 4H 50 1 OG 300.000 5000.000
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 1.29634401E+01 1.17954996E-02-4.04361488E-06 6.28771516E-10-3.65209867E-
 14 2
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 05 3
 1.28844447E-08-2.18165308E-12 2.85270691E+03 1.68774016E+01
 4
 IC4H7OOH 4/15/15 C 4H 80 2 OG 300.000 5000.000
 1386.000 41
 1.82897194E+01 1.67815784E-02-5.80668193E-06 9.08949180E-10-5.30513302E-
 14 2
 -1.82046522E+04-6.72111342E+01 1.31851762E-01 6.19561224E-02-4.99343877E-
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 2.09628211E-08-3.59717924E-12-1.21399925E+04 2.93905962E+01
 4
 IC3H6CO 03/03/95 THERMC 4H 60 1 OG 300.000 5000.000 1397.00
 41
 1.32548232E+01 1.40142787E-02-4.78910215E-06 7.42924342E-10-4.30737566E-
 14 2

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 05 3
 1.37243419E-08-2.40573132E-12-1.63939712E+04 1.38187714E+01
 4
 TC3H6OCHO 8/25/95 THERMC 4H 70 2 0G 300.000 5000.000 1394.00
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 14 2
 -2.75871941E+04-6.37271230E+01 3.70830259E-01 5.38475661E-02-3.82477565E-
 05 3
 1.32882237E-08-1.79228730E-12-2.18391262E+04 2.58142112E+01
 4
 TC3H6OHCHO 8/ 1/95 THERMC 4H 80 2 0G 300.000 5000.000 1396.00
 41
 1.70788996E+01 1.74005554E-02-5.93008112E-06 9.18860909E-10-5.32512140E-
 14 2
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 05 3
 1.37780428E-08-1.89068805E-12-4.80402638E+04 2.67836070E+01
 4
 C3H6OH2-1 8/ 9/ 4 THERMC 3H 70 1 0G 300.000 5000.000
 1392.000 31
 1.12222277E+01 1.36444398E-02-4.51406709E-06 7.10523275E-10-4.22690392E-
 14 2
 -1.75350136E+04-3.18911926E+01 1.09670360E+00 3.80727565E-02-2.75022497E-
 05 3
 1.07477493E-08-1.74895773E-12-1.40764487E+04 2.22475799E+01
 4
 TC3H6OH 8/ 9/ 4 THERMC 3H 70 1 0G 300.000 5000.000
 1392.000 31
 1.12222277E+01 1.36444398E-02-4.51406709E-06 7.10523275E-10-4.22690392E-
 14 2
 -1.75350136E+04-3.18911926E+01 1.09670360E+00 3.80727565E-02-2.75022497E-
 05 3
 1.07477493E-08-1.74895773E-12-1.40764487E+04 2.22475799E+01
 4
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 14 2
 -2.47298321E+04-3.13634050E+01 1.58376391E+00 3.16215366E-02-1.73664942E-
 05 3
 4.18927663E-09-2.79899620E-13-2.12643496E+04 1.88313766E+01
 4
 TC3H6O2CHO 8/ 2/95 THERMC 4H 70 3 0G 300.000 5000.000 1386.00
 41
 1.85534443E+01 1.68774389E-02-5.90752965E-06 9.31518085E-10-5.46345187E-
 14 2
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 1.38308104E-08-2.04190147E-12-2.27394154E+04 2.00751264E+01
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 TC3H6O2HCO 8/ 2/95 THERMC 4H 70 3 0G 300.000 5000.000 1387.00
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 14 2
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 05 3

1.58792094E-08-2.32209543E-12-2.24284673E+04 2.03680990E+01
4
IC3H5O2HCHO 8/2/95 THERMC 4H 70 3 0G 300.000 5000.000 1387.00
51
2.06288832E+01 1.48625539E-02-5.25305276E-06 8.33772951E-10-4.91277401E-
14 2
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05 3
1.63249918E-08-2.43462051E-12-1.63496250E+04 2.13687921E+01
4
CH2CCH2OH 9/ 8/95 THERMC 3H 50 1 0G 300.000 5000.000 1372.00
21
9.70702027E+00 1.13972660E-02-3.77993962E-06 5.75209277E-10-3.29229125E-
14 2
9.13212884E+03-2.25012933E+01 2.88422544E+00 2.42428071E-02-1.14152268E-
05 3
1.71775334E-09 1.42177454E-13 1.17935615E+04 1.52102335E+01
4
TC4H8CHO 9/ 7/95 THERMC 5H 90 1 0G 300.000 5000.000 1397.00
41
1.79663933E+01 1.94207117E-02-6.67409451E-06 1.03969221E-09-6.04702651E-
14 2
-1.33368585E+04-6.79819424E+01-9.58078294E-01 6.42003258E-02-4.70776827E-
05 3
1.75737698E-08-2.64896151E-12-6.86582501E+03 3.33781112E+01
4
O2C4H8CHO 9/ 7/95 THERMC 5H 90 3 0G 300.000 5000.000 1395.00
51
2.12629904E+01 2.14072282E-02-7.38342949E-06 1.15281523E-09-6.71508438E-
14 2
-3.16854524E+04-7.99828703E+01 1.91847699E+00 6.67245869E-02-4.80871046E-
05 3
1.78588690E-08-2.71163880E-12-2.49837984E+04 2.38577867E+01
4
O2HC4H8CO 9/ 7/95 THERMC 5H 90 3 0G 300.000 5000.000 1394.00
61
2.38219630E+01 1.91411448E-02-6.67919154E-06 1.05127303E-09-6.15876805E-
14 2
-3.23093973E+04-9.42580755E+01 1.82607262E+00 6.93466111E-02-4.93125140E-
05 3
1.69848340E-08-2.26117657E-12-2.46578311E+04 2.41167544E+01
4
C3H5OH T06/10C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
1
8.72477114E+00 1.63942712E-02-5.90852993E-06 9.53262253E-10-5.70318010E-
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05 3
-6.67818707E-08 2.80408237E-11-1.66413668E+04 1.35066359E+01-
1.48710589E+04 4
TIC4H7Q2-I 5/ 6/96 THERMC 4H 90 4 0G 300.000 5000.000
1400.000 71
2.33848631E+01 1.87070035E-02-6.44021945E-06 1.00428123E-09-5.84468189E-
14 2
-2.61180902E+04-8.76610135E+01 4.48426361E+00 6.61225007E-02-5.27349018E-
05 3
2.18215585E-08-3.66788946E-12-1.98906586E+04 1.26719614E+01
4

IIC4H7Q2-I 7/15/96 THERMC 4H 90 4 0G 300.000 5000.000
 1394.000 71
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 14 2
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 05 3
 1.49122008E-08-2.10978665E-12-1.68415495E+04 1.36228018E+01
 4
 IIC4H7Q2-T 5/27/15 C 4H 90 4 0G 300.000 5000.000
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 2.12381704E+01 2.09093209E-02-7.28830993E-06 1.14623127E-09-6.71107490E-
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 05 3
 4.25189720E-09 3.98800403E-13-1.59672252E+04 2.35098400E+01
 4
 C6H10 4/12/13 THERMC 6H 10 0 0G 300.000 5000.000
 1413.000 21
 1.60456030E+01 2.34774145E-02-7.85797929E-06 1.20200542E-09-6.90100029E-
 14 2
 2.11899382E+03-5.88452460E+01-1.01375402E+00 6.38242808E-02-4.40653860E-
 05 3
 1.58295163E-08-2.30830701E-12 7.94033696E+03 3.25056094E+01
 4
 C6H9-A 12/ 5/12 THERMC 6H 9 0 0G 300.000 5000.000
 1400.000 21
 1.70842767E+01 2.08842788E-02-7.14529004E-06 1.10943563E-09-6.43676989E-
 14 2
 2.01040204E+04-6.39326012E+01-2.66715213E+00 7.26196475E-02-6.05323920E-
 05 3
 2.66000571E-08-4.74613408E-12 2.64415017E+04 4.02220332E+01
 4
 C6H6 G 6/01C 6H 6 0 0G 200.000 6000.000
 1000.000 1
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 14 2
 4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-
 05 3
 -1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01
 9.96811598E+03 4
 C*CCJC*C 3/1/95 Z&B C 5H 7 0 0G 300.000 5000.000
 1388.000 21
 1.40879309E+01 1.62398907E-02-5.64768950E-06 8.86857524E-10-5.18698993E-
 14 2
 1.76798698E+04-5.13735038E+01-2.94595603E+00 5.68783623E-02-4.31336497E-
 05 3
 1.68169537E-08-2.67926433E-12 2.35156925E+04 3.98188778E+01
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 CC3H4 T12/81C 3H 4 0 0G 300.000 5000.00 1000.00
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 13 2
 0.30199051E+05-0.13378770E+02-0.24621047E-01 0.23197215E-01-0.18474357E-
 05 3
 -0.15927593E-07 0.86846155E-11 0.32334137E+05 0.22729762E+02 0.3332728
 E+05 4
 C4H3-I AB1/93C 4H 3 0 0G 300.000 3000.00 1000.00
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 13 2
 0.56600574E+05-0.19802597E+02 0.20830412E+01 0.40834274E-01-0.62159685E-
 04 3
 0.51679358E-07-0.17029184E-10 0.58005129E+05 0.13617462E+02
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 C4H612 A 8/83C 4H 6 0 0G 300.000 5000.000
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 14 2
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 05 3
 5.02139421E-09-3.67977164E-13 1.81439079E+04 2.02191143E+01
 4
 C6H5 T04/02C 6H 5 0 0G 200.000 6000.000 1000.
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 14 2
 3.55598475E+04-3.53735134E+01 2.10306633E-01 2.04745507E-02 5.89743006E-
 05 3
 -1.01534255E-07 4.47105660E-11 3.95468722E+04 2.52910455E+01
 4.08610970E+04 4
 C4H2 D11/99C 4H 2 0 0G 300.000 3000.000 1000.00
 1
 0.91576328E+01 0.55430518E-02-0.13591604E-05 0.18780075E-10 0.23189536E-
 13 2
 0.52588039E+05-0.23711460E+02 0.10543978E+01 0.41626960E-01-0.65871784E-
 04 3
 0.53257075E-07-0.16683162E-10 0.54185211E+05 0.14866591E+02
 4
 C4H3-N H6W/94C 4H 3 0 0G 300.000 3000.00 1000.00
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 0.54328279E+01 0.16860981E-01-0.94313109E-05 0.25703895E-08-0.27456309E-
 12 2
 0.61600680E+05-0.15673981E+01-0.31684113E+00 0.46912100E-01-0.68093810E-
 04 3
 0.53179921E-07-0.16523005E-10 0.62476199E+05 0.24622559E+02
 4
 C4H5-N H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00
 1
 0.98501978E+01 0.10779008E-01-0.13672125E-05-0.77200535E-09 0.18366314E-
 12 2
 0.38840301E+05-0.26001846E+02 0.16305321E+00 0.39830137E-01-0.34000128E-
 04 3
 0.15147233E-07-0.24665825E-11 0.41429766E+05 0.23536163E+02
 4
 C4H5-I H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00
 1
 0.10229092E+02 0.94850138E-02-0.90406445E-07-0.12596100E-08 0.24781468E-
 12 2
 0.34642812E+05-0.28564529E+02-0.19932900E-01 0.38005672E-01-0.27559450E-
 04 3
 0.77835551E-08 0.40209383E-12 0.37496223E+05 0.24394241E+02
 4
 CH3CHCHCO 12/ 6/13 THERMC 4H 50 1 0G 300.000 5000.000
 1396.000 11
 1.21043198E+01 1.28210886E-02-4.36704943E-06 6.75949572E-10-3.91295106E-
 14 2

-1.86544623E+03-3.77298604E+01 1.78215470E+00 3.99251915E-02-3.27534130E-
 05 3
 1.45472667E-08-2.65454288E-12 1.47887943E+03 1.67433588E+01
 4
 CH2CHCHCHO C 4H 50 1 0G 300.000 5000.000
 1385.000 11
 1.39299886E+01 1.13228814E-02-3.87393567E-06 6.02378620E-10-3.50120301E-
 14 2
 -2.39589898E+03-4.79026849E+01 4.51553480E-01 4.37530418E-02-3.37273602E-
 05 3
 1.31111496E-08-2.04732021E-12 2.14943141E+03 2.40835867E+01
 4
 C4H6O25 T 3/97C 4H 60 1 0G 200.000 5000.000 1000.0
 1
 8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-
 13 2
 -1.76177415E+04-2.32464750E+01 2.67053463E+00 4.92586420E-03 8.86967406E-
 05 3
 -1.26219194E-07 5.23991321E-11-1.46572472E+04 1.45722395E+01-
 1.30831522E+04 4
 C2H3CHOCH2 C 4H 60 1 0G 300.000 5000.000
 1431.000 11
 1.26762790E+01 1.40819509E-02-4.63473868E-06 7.01090838E-10-3.99438277E-
 14 2
 -4.08065264E+03-4.22515995E+01-3.59388437E+00 5.79063450E-02-4.97163294E-
 05 3
 2.15818682E-08-3.69199072E-12 8.58852628E+02 4.28475443E+01
 4
 C4H5-2 12/ 6/13 THERMC 4H 5 0 0G 300.000 5000.000
 2021.000 21
 8.67673333E+00 1.42789766E-02-5.26476298E-06 8.62021059E-10-5.19571720E-
 14 2
 3.21729573E+04-2.14573334E+01 2.74016965E+00 2.31992086E-02-7.25585511E-
 06 3
 -1.04665455E-09 6.55179692E-13 3.46243943E+04 1.20689663E+01
 4
 C4H6-2 12/ 6/13 THERMC 4H 6 0 0G 300.000 5000.000
 1525.000 21
 1.17580664E+01 1.36774582E-02-4.88993888E-06 7.81986154E-10-4.63144942E-
 14 2
 1.13714894E+04-4.11767591E+01 2.34411768E+00 2.27019178E-02 2.71441556E-
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 4
 C4H6O23 T 3/97C 4H 60 1 0G 200.000 5000.000 1000.0
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 13 2
 -1.32392815E+04-2.32464750E+01 2.67053463E+00 4.92586420E-03 8.86967406E-
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 1.30831522E+04 4
 CH3CHCHCHO C 4H 60 1 0G 300.000 5000.000
 1390.000 21
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 14 2
 -2.02867889E+04-4.48216674E+01 7.26850107E-01 4.38069262E-02-3.21167642E-
 05 3

1.23413678E-08-1.96193679E-12-1.59649030E+04 2.22276969E+01
 4
 C4H4O T03/97C 4H 40 1 0G 200.000 6000.0 1000.0
 1
 9.38935003E+00 1.40291241E-02-5.07755110E-06 8.24137332E-10-4.95319963E-
 14 2
 -8.68241814E+03-2.79162920E+01 8.47469463E-01 1.31773796E-02 5.99735901E-
 05 3
 -9.71562904E-08 4.22733796E-11-5.36785445E+03 2.14945172E+01-
 4.17166616E+03 4
 H2CC L12/89H 2C 2 0 0G 200.000 6000.000
 1000.000 1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-
 13 2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-
 05 3
 -0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01
 0.49887266E+05 4
 H2C4O 120189H 2C 40 1 G 0300.00 4000.00 1000.00
 1
 0.01026888E+03 0.04896164E-01-0.04885081E-05-0.02708566E-08 0.05107013E-
 12 2
 0.02346903E+06-0.02815985E+03 0.04810971E+02 0.01313999E+00 0.09865073E-
 05 3
 -0.06120720E-07 0.01640003E-10 0.02545803E+06 0.02113424E+02
 4
 C6H2 P 1/93C 6H 2 0 0G 300.000 3000.00 1000.00
 1
 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-
 14 2
 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-
 03 3
 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02
 4
 C6H3 H6W/94C 6H 3 0 0G 300.000 3000.00 1000.00
 1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-
 12 2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-
 04 3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02
 4
 L-C6H4 H6W/94C 6H 4 0 0G 300.000 3000.00 1000.00
 1
 0.12715182E+02 0.13839662E-01-0.43765440E-05 0.31541636E-09 0.46619026E-
 13 2
 0.57031148E+05-0.39464600E+02 0.29590225E+00 0.58053318E-01-0.67766756E-
 04 3
 0.43376762E-07-0.11418864E-10 0.60001371E+05 0.22318970E+02
 4
 C-C6H4 H6W/94C 6H 4 0 0G 300.000 3000.00 1000.00
 1
 0.13849209E+02 0.78807920E-02 0.18243836E-05-0.21169166E-08 0.37459977E-
 12 2
 0.47446340E+05-0.50404953E+02-0.30991268E+01 0.54030564E-01-0.40839004E-
 04 3
 0.10738837E-07 0.98078490E-12 0.52205711E+05 0.37415207E+02
 4

C6H5OH L 4/84C 6H 60 1 0G 300.000 5000.000 1000.
1
0.14912073E+02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-
13 2
-0.18375199E+05-0.55924103E+02-0.16956539E+01 0.52271299E-01-0.72024050E-
05 3
-0.35859603E-07 0.20449073E-10-0.13284121E+05 0.32542160E+02-
0.11594207E+05 4
C6H5O T05/02C 6H 50 1 0G 200.000 6000.000 1000.
1
1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-
14 2
2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-
05 3
-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01
6.49467016E+03 4
P-C6H4O2 AK0405C 6H 40 2 0G 270.000 3000.000 1370.00
1
1.23423732E+01 2.40612690E-02-1.16565184E-05 2.71393504E-09-2.47643065E-
13 2
-2.06185312E+04-4.08244024E+01-2.43170113E+00 6.87937608E-02-6.41382837E-
05 3
3.08126855E-08-5.99832072E-12-1.65696994E+04 3.48309430E+01
4
P-C6H3O2 AK0505C 6H 30 2 0G 270.000 3000.000 1290.00
1
1.22963699E+01 2.15055142E-02-1.07516136E-05 2.57528163E-09-2.41023652E-
13 2
1.15428998E+04-3.72584002E+01-1.57852347E+00 6.55376473E-02-6.50308721E-
05 3
3.32026554E-08-6.86665555E-12 1.51750093E+04 3.31518638E+01
4
O-C6H4O2 AK0405C 6H 40 2 0G 270.000 3000.000 1370.00
1
1.23614349E+01 2.40491397E-02-1.16529057E-05 2.71332785E-09-2.47593219E-
13 2
-1.67079717E+04-4.00310857E+01-2.36179712E+00 6.86058343E-02-6.39129516E-
05 3
3.06903009E-08-5.97357785E-12-1.26704431E+04 3.53724482E+01
4
C5H5 TAK0505C 5H 5 0 0G 298.150 3500.000 969.35
1
1.33675715E+00 3.24793912E-02-1.67587774E-05 4.03514137E-09-3.70739036E-
13 2
3.00730524E+04 1.60315806E+01-3.97555452E+00 7.41370991E-02-1.11803345E-
04 3
9.04628776E-08-2.80999747E-11 3.01769405E+04 3.67153636E+01
4
C5H6 T 1/90C 5H 6 0 0G 200.000 6000.000 1000.
1
0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-
13 2
0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-
04 3
-0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02
0.16152485E+05 4
C5H5OH 5/ 2/91 THE.MC 5H 60 1 0G 300.000 5000.000
1398.000 11

1.53433477E+01 1.50754059E-02-5.13553582E-06 7.95807816E-10-4.61311517E-
14 2
-1.19645453E+04-5.85204430E+01-4.26822012E+00 6.62446749E-02-5.68494038E-
05 3
2.46858526E-08-4.26820696E-12-5.75581338E+03 4.47962850E+01
4
C5H4O T 8/99C 5H 40 1 0G 200.000 6000.000 1000.
1
1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-
14 2
1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-
06 3
-2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01
6.64245999E+03 4
C5H5O 5/16/90 THERMC 5H 50 1 0G 300.000 5000.000
1392.000 01
1.48322894E+01 1.40483376E-02-4.92302051E-06 7.77041219E-10-4.56103939E-
14 2
1.45523665E+04-5.73228191E+01-2.83112840E+00 5.67277287E-02-4.44757303E-
05 3
1.74924447E-08-2.76004847E-12 2.04992154E+04 3.69634411E+01
4
C5H4OH T 8/99C 5H 50 1 0G 200.000 6000.000 1000.
1
1.33741248E+01 1.51996469E-02-5.45685046E-06 8.80944866E-10-5.27493258E-
14 2
2.20358027E+03-4.59569069E+01-1.28398054E+00 4.90298511E-02-1.35844414E-
05 3
-2.92983743E-08 1.90820619E-11 6.37364803E+03 3.08073591E+01
8.00114499E+03 4
C6H5OO 3/26/ 9 THERMC 6H 50 2 0G 300.000 5000.000
1403.000 11
1.67078262E+01 1.62326229E-02-5.47969630E-06 8.43510060E-10-4.86562431E-
14 2
8.14242915E+03-6.08346973E+01-2.99164672E+00 7.03857150E-02-6.34400574E-
05 3
2.91548920E-08-5.30706938E-12 1.41320240E+04 4.20142955E+01
4
C6H5OOH 3/26/ 9 THERMC 6H 60 2 0G 300.000 5000.000
1404.000 21
1.92317474E+01 1.63154699E-02-5.53448904E-06 8.55059974E-10-4.94583790E-
14 2
-1.01971012E+04-7.61674471E+01-4.03105975E+00 7.96101888E-02-7.21655013E-
05 3
3.27610696E-08-5.85584239E-12-3.10973017E+03 4.54324978E+01
4
C6H4OH 4/ 9/ 9 THERMC 6H 50 1 0G 300.000 5000.000
1402.000 11
1.73187560E+01 1.36366984E-02-4.68316332E-06 7.29071204E-10-4.23805358E-
14 2
1.14990276E+04-6.89986593E+01-5.99875435E+00 8.59063379E-02-9.12525636E-
05 3
4.72275890E-08-9.35576749E-12 1.78621926E+04 4.99931427E+01
4
OC6H4OH 4/ 9/ 9 THERMC 6H 50 2 0G 300.000 5000.000
1403.000 11
2.22718210E+01 1.21038561E-02-4.18429526E-06 6.54475399E-10-3.81746504E-
14 2

-2.34827539E+04-9.61035467E+01-8.02205657E+00 1.09403210E-01-1.23489276E-
 04 3
 6.56286805E-08-1.31527870E-11-1.55949156E+04 5.72175202E+01
 4
 P-OC6H5OJ WKM C 60 2H 5 0G 300.000 5000.000
 1400.000 01
 1.82799770E+01 1.59280974E-02-5.50765220E-06 8.61649836E-10-5.02677539E-
 14 2
 -6.25907994E+01-7.25809444E+01-3.29683290E+00 7.27365977E-02-6.36158220E-
 05 3
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 4
 O-OC6H5OJ WKM C 60 2H 5 0G 300.000 5000.000
 1400.000 01
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 14 2
 -1.72770226E+02-7.28742484E+01-2.65459198E+00 7.17179095E-02-6.31552372E-
 05 3
 2.81132946E-08-4.97463333E-12 6.45283150E+03 3.81123139E+01
 4
 C#CC*CCJ GLAR C 5H 5 0 0G 300.000 5000.000
 1396.000 11
 1.41230912E+01 1.14233190E-02-3.95851276E-06 6.20128961E-10-3.62097887E-
 14 2
 4.25158384E+04-5.02942871E+01-6.16143558E-01 5.06466579E-02-4.48561743E-
 05 3
 2.02459419E-08-3.64542145E-12 4.71532377E+04 2.71623299E+01
 4
 C5H6-L 2/ 5/ 9 THERMC 5H 6 0 0G 300.000 5000.000
 1372.000 21
 1.29600892E+01 1.48953758E-02-5.23622902E-06 8.27916389E-10-4.86464523E-
 14 2
 2.38180800E+04-4.25312093E+01 3.58448213E+00 3.24459626E-02-1.70150991E-
 05 3
 4.22715914E-09-4.18452556E-13 2.76514681E+04 9.60644208E+00
 4
 CJ*CC*CC*O 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000
 1396.000 21
 1.62360823E+01 1.18297101E-02-4.11454219E-06 6.46026823E-10-3.77767639E-
 14 2
 1.93499885E+04-5.83498817E+01-5.06628841E-01 6.04671965E-02-5.97396749E-
 05 3
 2.96804228E-08-5.76240010E-12 2.42765544E+04 2.82994148E+01
 4
 C*CC*CCJ*O 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000
 1399.000 11
 1.53178248E+01 1.27352911E-02-4.35882964E-06 6.76912763E-10-3.92771371E-
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 7.60582726E+03-5.43599625E+01-2.18492198E-01 5.92100223E-02-5.89241174E-
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 2.97411920E-08-5.85244770E-12 1.20600764E+04 2.55968530E+01
 4
 CJ*CC*O 4/ 8/94 THERMC 3H 30 1 0G 300.000 5000.000
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 14 2
 1.51410162E+04-3.01266033E+01 1.46654466E+00 3.23390476E-02-3.05588208E-
 05 3

1.44081861E-08-2.65600505E-12 1.78850058E+04 1.80850321E+01
 4
 C5H30 TAK0905C 5H 30 1 OG 300.000 3500.000 1500.00
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 14 2
 2.89592010E+04-4.07548249E+01-3.03242604E+00 5.43937201E-02-4.95018348E-
 05 3
 2.25523751E-08-4.10727920E-12 3.35644081E+04 3.78374823E+01
 4
 C5H7 1/22/ 9 WKM C 5H 7 0 OG 300.000 5000.000
 1377.000 31
 1.36630213E+01 1.68061358E-02-5.98746539E-06 9.55341072E-10-5.64951981E-
 14 2
 1.27238941E+04-5.46331286E+01-6.75118368E+00 6.06461693E-02-4.01260152E-
 05 3
 1.22051562E-08-1.33459844E-12 2.01365277E+04 5.62694938E+01
 4
 OC5H70 1/22/ 9 WKM C 5H 70 2 OG 300.000 5000.000
 1375.000 31
 1.65416953E+01 1.86677673E-02-6.44836048E-06 1.00787611E-09-5.87521858E-
 14 2
 -2.82017168E+04-5.47258181E+01 4.88394767E+00 4.03401300E-02-1.97774150E-
 05 3
 3.68903501E-09-3.40202384E-14-2.35295942E+04 9.97070337E+00
 4
 C*CCJC*COH 10/6/95 Z&B C 5H 70 1 OG 300.000 5000.000
 1397.000 31
 1.67465815E+01 1.58357240E-02-5.44954706E-06 8.49881387E-10-4.94743246E-
 14 2
 -4.30972870E+03-6.19378748E+01-2.91175436E+00 6.69362484E-02-5.71603047E-
 05 3
 2.48753749E-08-4.33243894E-12 1.96441523E+03 4.17454344E+01
 4
 C*CC*CCJ Z&B C 5H 7 0 OG 300.000 5000.000
 1386.000 21
 1.47302883E+01 1.59030900E-02-5.57729508E-06 8.80604825E-10-5.16963733E-
 14 2
 1.74050791E+04-5.42670706E+01-1.60087476E+00 5.38764703E-02-3.96302225E-
 05 3
 1.49599474E-08-2.31995284E-12 2.31199746E+04 3.35492960E+01
 4
 C*CC*CC 3/1/95 Z&B C 5H 8 0 OG 300.000 5000.000
 1395.000 21
 1.41303131E+01 1.81877961E-02-6.19208788E-06 9.58333792E-10-5.54785472E-
 14 2
 2.25907168E+03-5.11705577E+01-1.19376866E+00 5.65474329E-02-4.39472481E-
 05 3
 1.82341266E-08-3.12226566E-12 7.36084709E+03 3.02808980E+01
 4
 C*CC*CCOH 1/23/ 9 WKM C 5H 80 1 OG 300.000 5000.000
 1396.000 31
 1.63079670E+01 1.79957763E-02-6.03115896E-06 9.23992259E-10-5.31254053E-
 14 2
 -1.58204603E+04-5.84137244E+01-5.31488384E-01 6.06983915E-02-4.81499862E-
 05 3
 2.00308244E-08-3.38987282E-12-1.03301302E+04 3.07961436E+01
 4

C*CCJC*O Z&B C 4H 50 1 0G 300.000 5000.000
1385.000 11
1.22833215E+01 1.26428506E-02-4.31034879E-06 6.68415867E-10-3.87693974E-
14 2
1.86818728E+03-3.84807909E+01-4.83886977E-01 4.23431670E-02-3.05389089E-
05 3
1.11441978E-08-1.63863920E-12 6.28635090E+03 3.00860103E+01
4
OC4H6O 1/23/ 9 WKM C 4H 60 2 0G 300.000 5000.000
1382.000 31
1.41894774E+01 1.53345510E-02-5.24594862E-06 8.14655154E-10-4.72759368E-
14 2
-4.10001835E+04-4.43771751E+01 4.21628848E+00 3.57422725E-02-2.04226185E-
05 3
5.63821367E-09-5.88888993E-13-3.72055911E+04 1.02814620E+01
4
OC4H5O 1/23/ 9 WKM C 4H 50 2 0G 300.000 5000.000
1388.000 21
1.32138775E+01 1.37339051E-02-4.62639517E-06 7.10941370E-10-4.09538499E-
14 2
-2.16535271E+04-3.64185255E+01 4.60550978E+00 3.30498712E-02-2.13102363E-
05 3
7.37021089E-09-1.08289438E-12-1.85460831E+04 1.01599453E+01
4
HOC*CC*O 1/26/ 9 WKM C 3H 40 2 0G 300.000 5000.000
1413.000 21
1.66505478E+01 6.11745137E-03-2.09080785E-06 3.24985683E-10-1.88875073E-
14 2
-3.82179939E+04-6.36794754E+01-2.01837189E+00 6.26539783E-02-6.73359280E-
05 3
3.39430425E-08-6.48917648E-12-3.31367523E+04 3.18162860E+01
4
HOC*CCJ*O 1/26/ 9 WKM C 3H 30 2 0G 300.000 5000.000
1414.000 11
1.52720985E+01 5.02586331E-03-1.68408578E-06 2.58390706E-10-1.48849424E-
14 2
-1.98506828E+04-5.54641734E+01 6.07270082E-01 4.96011303E-02-5.32300885E-
05 3
2.68392951E-08-5.13094510E-12-1.58814562E+04 1.94817133E+01
4
C2H2OH H 3C 20 1 0G 300.000 5000.000
1401.000 11
8.20268447E+00 5.92989165E-03-1.99194448E-06 3.05794341E-10-1.76114732E-
14 2
1.24881328E+04-1.89670436E+01 6.41642616E-01 2.61903633E-02-2.30385370E-
05 3
1.02804704E-08-1.81971416E-12 1.48276951E+04 2.06750999E+01
4
O2CCHOOJ Z&B C 2H 10 4 0G 300.000 5000.000
1682.000 01
1.09910849E+01 7.46985861E-03-2.75568271E-06 4.51353051E-10-2.72108652E-
14 2
-3.51335323E+04-2.11652231E+01 8.91497688E+00 8.60571847E-03 5.24416766E-
07 3
-2.79301331E-09 7.62963051E-13-3.40867754E+04-8.72978273E+00
4
HCOH MAR94 C 1H 20 1 0G 300. 5000. 1398.
1

9.18749272E+00 1.52011152E-03-6.27603516E-07 1.09727989E-10-6.89655128E-
 15 2
 7.81364593E+03-2.73434214E+01-2.82157421E+00 3.57331702E-02-3.80861580E-
 05 3
 1.86205951E-08-3.45957838E-12 1.12956672E+04 3.48487757E+01
 4
 C2H3OH 2/ 3/ 9 THERMC 2H 40 1 0G 300.000 5000.000
 1410.000 11
 8.32598158E+00 8.03387281E-03-2.63928405E-06 3.98410726E-10-2.26551155E-
 14 2
 -1.83221436E+04-2.02080305E+01-1.27972260E-01 3.38506073E-02-3.30644935E-
 05 3
 1.64858739E-08-3.19935455E-12-1.59914544E+04 2.30438601E+01
 4
 O2CH2CHO BOZ_03C 2H 30 3 0G 300.000 5000.000
 1393.000 01
 1.11807543E+01 9.14479256E-03-3.15089833E-06 4.91944238E-10-2.86639180E-
 14 2
 -1.55790331E+04-2.87892740E+01-1.29465843E+00 4.44936393E-02-4.26577074E-
 05 3
 2.07391950E-08-3.96828771E-12-1.18275628E+04 3.60778797E+01
 4
 HO2CH2CO BOZ_03C 2H 30 3 0G 300.000 5000.000
 1386.000 01
 1.04146322E+01 1.12680116E-02-5.17494839E-06 1.00333285E-09-6.68165911E-
 14 2
 -1.40955672E+04-2.27894400E+01 2.22681686E+00 3.56781380E-02-3.26401909E-
 05 3
 1.47651988E-08-2.64794380E-12-1.18735095E+04 1.91581197E+01
 4
 SC3H4OH 3/28/13 C 3H 50 1 0G 300.000 5000.000
 1407.000 21
 1.20968484E+01 9.43976596E-03-3.10773897E-06 4.69609188E-10-2.67165710E-
 14 2
 -3.85854894E+02-3.76795997E+01 1.72870561E+00 4.41015870E-02-4.72013860E-
 05 3
 2.52073596E-08-5.13375710E-12 2.22720503E+03 1.43928257E+01
 4
 PC3H4OH-2 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1403.000 21
 1.07164095E+01 1.06066461E-02-3.51374060E-06 5.33713932E-10-3.04901511E-
 14 2
 4.98486803E+03-2.98329329E+01 1.42757363E+00 3.64825569E-02-3.18007132E-
 05 3
 1.46914605E-08-2.72331227E-12 7.80342663E+03 1.85890339E+01
 4
 SC3H5OH 2/ 3/ 9 C 3H 60 1 0G 300.000 5000.000
 1404.000 21
 1.11222064E+01 1.27745410E-02-4.25315532E-06 6.48216484E-10-3.71190850E-
 14 2
 -2.36690795E+04-3.41335182E+01-3.53977226E-02 4.34969453E-02-3.74479918E-
 05 3
 1.70906074E-08-3.13775054E-12-2.02502608E+04 2.41528201E+01
 4
 IC4H8OH-IT C 4H 90 1 0G 300.000 5000.000
 1391.000 41
 1.29136746E+01 2.06583409E-02-6.98445966E-06 1.07562552E-09-6.20443876E-
 14 2

-1.81394866E+04-3.84972088E+01 3.05275715E+00 3.93926461E-02-1.90686417E-
 05 3
 3.86408022E-09-1.48005244E-13-1.42263749E+04 1.60840537E+01
 4
 IC4H8OH-TI C 4H 90 1 0G 300.000 5000.000
 1402.000 41
 1.46323607E+01 1.88895981E-02-6.30561450E-06 9.62474230E-10-5.51640163E-
 14 2
 -1.87976018E+04-4.93218793E+01 2.33169342E+00 5.13017040E-02-4.02698872E-
 05 3
 1.75150405E-08-3.16001727E-12-1.48318978E+04 1.55368130E+01
 4
 IQJC4H8OH L 2/00C 4H 90 3 0G 300.000 5000.000
 1410.000 51
 2.11752212E+01 1.75144254E-02-5.73227292E-06 8.63386596E-10-4.90282414E-
 14 2
 -3.98881576E+04-8.19187015E+01 1.81448831E+00 7.47452750E-02-7.10895172E-
 05 3
 3.44973679E-08-6.54646593E-12-3.44023586E+04 1.77380434E+01
 4
 IQC4H8OT C 4H 90 3 0G 300.000 5000.000
 1405.000 51
 2.04823628E+01 1.82966721E-02-6.04413378E-06 9.16380548E-10-5.22866551E-
 14 2
 -2.94287153E+04-7.53563247E+01 3.72211529E+00 6.42864861E-02-5.52809053E-
 05 3
 2.50036630E-08-4.53471908E-12-2.43110525E+04 1.21981167E+01
 4
 IQC4H7OHT C 4H 90 3 0G 300.000 5000.000
 1413.000 61
 2.19945886E+01 1.62011186E-02-5.23758492E-06 7.81898296E-10-4.41125515E-
 14 2
 -3.07383725E+04-8.16613568E+01 3.58900054E+00 7.25591129E-02-7.14080484E-
 05 3
 3.55250907E-08-6.84991795E-12-2.57241250E+04 1.23766657E+01
 4
 TQJC4H8OH C 4H 90 3 0G 300.000 5000.000
 1415.000 51
 2.29681617E+01 1.65162786E-02-5.50247318E-06 8.39335285E-10-4.81030625E-
 14 2
 -4.10051460E+04-9.34897892E+01-6.43419503E-01 8.49131517E-02-8.17210578E-
 05 3
 3.90979927E-08-7.27092842E-12-3.42375932E+04 2.84394025E+01
 4
 TQC4H8OI C 4H 90 3 0G 300.000 5000.000
 1411.000 51
 2.13200701E+01 1.80489663E-02-6.06124072E-06 9.29740751E-10-5.34977374E-
 14 2
 -3.12966663E+04-8.20046659E+01 7.45747835E-02 7.46499596E-02-6.42255048E-
 05 3
 2.80908988E-08-4.87692045E-12-2.47182737E+04 2.94511549E+01
 4
 TQC4H7OHI L 2/00C 4H 90 3 0G 300.000 5000.000
 1404.000 61
 2.08281225E+01 1.81675094E-02-6.12943202E-06 9.43194119E-10-5.43937008E-
 14 2
 -3.37386684E+04-7.74823720E+01 2.55843807E+00 6.37086077E-02-4.97169945E-
 05 3

1.99225109E-08-3.21373436E-12-2.77526909E+04 1.95001368E+01
 4
 QC4H7OHP C 4H 90 3 OG 300.000 5000.000
 1416.000 61
 2.43481084E+01 1.50316366E-02-5.01788017E-06 7.66774357E-10-4.40093220E-
 14 2
 -3.31922320E+04-9.68211106E+01-1.27864186E+00 8.94492926E-02-8.78565423E-
 05 3
 4.22110919E-08-7.83450876E-12-2.58975226E+04 3.53963909E+01
 4
 CCY(CCO)COH C 4H 80 2 OG 300.000 5000.000
 1412.000 31
 1.91884885E+01 1.56255714E-02-5.22569800E-06 7.99171074E-10-4.58832445E-
 14 2
 -4.71120302E+04-7.84579023E+01-7.10048774E+00 9.53371808E-02-9.78701612E-
 05 3
 4.90005646E-08-9.41685766E-12-3.98987202E+04 5.60924667E+01
 4
 C2CY(COC)OH C 4H 80 2 OG 300.000 5000.000
 1393.000 31
 1.56829970E+01 1.92910506E-02-6.63718495E-06 1.03441014E-09-6.01715267E-
 14 2
 -4.10598236E+04-5.85686221E+01 5.92324183E-01 5.52429007E-02-4.02419018E-
 05 3
 1.57152217E-08-2.57388393E-12-3.58241476E+04 2.23378086E+01
 4
 CCY(CCOC)OH L 2/00C 4H 80 2 OG 300.000 5000.000
 1404.000 21
 1.43404718E+01 1.98311504E-02-6.60657660E-06 1.00779570E-09-5.77614335E-
 14 2
 -4.30959414E+04-5.30535015E+01-2.84914896E+00 6.23736856E-02-4.70326536E-
 05 3
 1.84908286E-08-2.94976027E-12-3.74257004E+04 3.83163588E+01
 4
 IC3H6OHCHO C 4H 80 2 OG 300.000 5000.000
 1393.000 41
 1.60254376E+01 1.85402212E-02-6.36973877E-06 9.91732739E-10-5.76472640E-
 14 2
 -5.50198923E+04-5.83074874E+01 1.84080874E+00 5.29601347E-02-3.94261774E-
 05 3
 1.59063430E-08-2.69565279E-12-5.01437169E+04 1.75482756E+01
 4
 CH3COCOHH C 3H 60 3 OG 300.000 5000.000
 1405.000 41
 1.61208655E+01 1.25067303E-02-4.10793603E-06 6.20553031E-10-3.53216368E-
 14 2
 -4.09312648E+04-5.27056280E+01 4.22993148E+00 4.45552095E-02-3.76424204E-
 05 3
 1.66306528E-08-2.94629936E-12-3.72634997E+04 9.58272910E+00
 4
 IC3H5COHQ C 4H 80 3 OG 300.000 5000.000
 1504.000 51
 2.07387831E+01 1.58360934E-02-5.27614462E-06 8.05932218E-10-4.62682425E-
 14 2
 -4.41821241E+04-7.94239893E+01 2.64360992E+00 5.72485066E-02-3.95907807E-
 05 3
 1.27775635E-08-1.47241476E-12-3.80099993E+04 1.77322273E+01
 4

IC3H5Q C 3H 60 2 0G 300.000 5000.000
 1397.000 31
 1.43424294E+01 1.28053632E-02-4.40584813E-06 6.86848148E-10-3.99675209E-14 2
 -1.65261025E+04-4.89934539E+01 1.32903007E+00 4.49170722E-02-3.51235127E-05 3
 1.41982181E-08-2.33335008E-12-1.21898396E+04 2.02696565E+01
 4
 TQC4H7OHIO2 C 4H 90 5 0G 300.000 5000.000
 1402.000 71
 2.82564819E+01 1.66969871E-02-5.67314614E-06 8.78350442E-10-5.09090253E-14 2
 -5.66017464E+04-1.15147927E+02 3.17336206E+00 7.94005900E-02-6.51165712E-05 3
 2.62035931E-08-4.13406290E-12-4.84943162E+04 1.77867184E+01
 4
 TQC4H7OHIQ-I C 4H 90 5 0G 300.000 5000.000
 1384.000 71
 2.88466964E+01 1.66289773E-02-5.74301906E-06 8.98791324E-10-5.24794891E-14 2
 -4.69249234E+04-1.19117836E+02 6.09881562E+00 6.93745451E-02-5.12049498E-05 3
 1.81276221E-08-2.46329781E-12-3.91393707E+04 2.93862639E+00
 4
 TQC4H7OHIQ-P C 4H 90 5 0G 300.000 5000.000
 1400.000 81
 2.81439191E+01 1.63524649E-02-5.54998081E-06 8.58603978E-10-4.97359401E-14 2
 -4.84502814E+04-1.11572783E+02 3.36947511E+00 7.96855226E-02-6.74365765E-05 3
 2.82233283E-08-4.65270820E-12-4.05567534E+04 1.92726029E+01
 4
 CH2CQCOHQ 7/ 1/14 C 3H 60 5 0G 300.000 5000.000
 1418.000 61
 3.86574091E+01 4.83815026E-04-2.10413843E-07 3.81490832E-11-2.46187754E-15 2
 -6.56392184E+04-1.61083579E+02-1.61171759E+01 1.78866440E-01-2.16751308E-04 3
 1.15450289E-07-2.27163078E-11-5.21165145E+04 1.14441286E+02
 4
 COHQCYC (COC) C 4H 80 4 0G 300.000 5000.000
 1319.000 51
 2.44599226E+01 1.64187782E-02-5.74024372E-06 9.05710407E-10-5.31829152E-14 2
 -6.01811228E+04-1.02049722E+02 2.40687943E+00 5.95180442E-02-3.16913659E-05 3
 4.23694824E-09 8.42033474E-13-5.19694864E+04 1.88941416E+01
 4
 QCYC (CCOC) OH C 4H 80 4 0G 300.000 5000.000
 1411.000 41
 2.20860197E+01 1.83743733E-02-6.29478769E-06 9.78787994E-10-5.68621317E-14 2
 -5.89652037E+04-8.64964494E+01-2.09099972E+00 8.02656739E-02-6.69756245E-05 3
 2.79282034E-08-4.60981823E-12-5.12529252E+04 4.11897260E+01
 4
 TQC4H7OHTO2 C 4H 90 5 0G 300.000 5000.000
 1402.000 71

2.82564819E+01 1.66969871E-02-5.67314614E-06 8.78350442E-10-5.09090253E-
 14 2
 -5.66017464E+04-1.15147927E+02 3.17336206E+00 7.94005900E-02-6.51165712E-
 05 3
 2.62035931E-08-4.13406290E-12-4.84943162E+04 1.77867184E+01
 4
 HOCOCQ(CH3)2 C 4H 80 4 OG 300.000 5000.000
 1380.000 61
 2.28935401E+01 1.78627606E-02-6.34627520E-06 1.01068546E-09-5.96885712E-
 14 2
 -8.05400680E+04-9.08953779E+01 1.56326363E+00 6.77165643E-02-5.14600149E-
 05 3
 1.99184629E-08-3.16007445E-12-7.30943302E+04 2.37255421E+01
 4
 IQC4H7OHTO2 C 4H 90 5 OG 300.000 5000.000
 1389.000 71
 2.41720261E+01 2.09397176E-02-7.29061406E-06 1.14554056E-09-6.70217517E-
 14 2
 -5.04772118E+04-8.95996685E+01 3.83287364E+00 6.90926177E-02-5.15031144E-
 05 3
 1.99235553E-08-3.17456897E-12-4.34442789E+04 1.94648622E+01
 4
 IQC4H7OHTQ-P C 4H 90 5 OG 300.000 5000.000
 1391.000 81
 2.45769593E+01 2.01889393E-02-7.03584537E-06 1.10623327E-09-6.47523225E-
 14 2
 -4.25783112E+04-9.05052742E+01 3.45242802E+00 7.14541224E-02-5.54616790E-
 05 3
 2.22754676E-08-3.66067450E-12-3.54133076E+04 2.23024492E+01
 4
 IQC4H8OTQ-I C 4H 90 5 OG 300.000 5000.000
 1386.000 71
 2.53249383E+01 2.00634820E-02-7.01249558E-06 1.10475030E-09-6.47561724E-
 14 2
 -4.09610593E+04-9.73592779E+01 5.90219800E+00 6.26952142E-02-4.17351838E-
 05 3
 1.35422162E-08-1.71169663E-12-3.39620020E+04 7.89290087E+00
 4
 CH2COHCH2OOH C 3H 60 3 OG 300.000 5000.000
 1398.000 41
 1.87971268E+01 1.12783442E-02-3.90789058E-06 6.12064651E-10-3.57305453E-
 14 2
 -3.61154867E+04-6.94914300E+01-3.89823383E-01 7.01531131E-02-7.42036788E-
 05 3
 3.84181056E-08-7.63555985E-12-3.07879938E+04 2.86873505E+01
 4
 CH2C(CH2OOH)2 C 4H 80 4 OG 300.000 5000.000
 1386.000 61
 2.50360805E+01 1.60230197E-02-5.70704966E-06 9.10412038E-10-5.38294659E-
 14 2
 -2.84196401E+04-9.60241308E+01 2.16408482E-01 8.25572149E-02-7.64540445E-
 05 3
 3.58211787E-08-6.67718658E-12-2.05694845E+04 3.43888367E+01
 4
 CO(CH2OOH)2 C 3H 60 5 OG 300.000 5000.000
 1393.000 61
 2.43376341E+01 1.14074110E-02-4.08931881E-06 6.55183244E-10-3.88570518E-
 14 2

-5.16862647E+04-9.01518175E+01-2.47626577E+00 8.93736793E-02-9.25891121E-05 3
 4.63168490E-08-8.93300309E-12-4.38924057E+04 4.84479477E+01
 4
 CHOC(CH3)OHCH2O C 4H 80 4 OG 300.000 5000.000
 1383.000 61
 2.24480753E+01 1.78753902E-02-6.26904597E-06 9.90084046E-10-5.81417382E-14 2
 -6.55093075E+04-8.56747327E+01 2.40933530E+00 6.13326038E-02-4.03874986E-05 3
 1.22738404E-08-1.32997480E-12-5.83049516E+04 2.29870742E+01
 4
 CH3COCHO C 3H 40 2 OG 300.000 5000.000
 1381.000 21
 1.14371190E+01 1.06773624E-02-3.68967757E-06 5.77006752E-10-3.36532201E-14 2
 -3.78079398E+04-3.25054087E+01 2.08731049E+00 3.09032484E-02-1.98794164E-05 3
 6.26174519E-09-7.69945504E-13-3.43989451E+04 1.82839639E+01
 4
 IC4H7O2 L 2/00C 4H 70 2 OG 300.000 5000.000
 1404.000 31
 1.45791608E+01 1.62136068E-02-5.26957103E-06 7.90454323E-10-4.47755051E-14 2
 -1.20848042E+03-4.56459433E+01 1.43532045E+00 4.89026570E-02-3.63600970E-05 3
 1.41906420E-08-2.24557878E-12 3.09284623E+03 2.41320196E+01
 4
 IC4H7OOIC4H7 C 8H 140 2 OG 300.000 5000.000
 1390.000 71
 2.80447245E+01 3.27505220E-02-1.13220177E-05 1.77027767E-09-1.03211988E-13 2
 -1.72683337E+04-1.15134796E+02-2.07881710E-01 1.04075647E-01-8.33973077E-05 3
 3.60897624E-08-6.47906520E-12-7.79062693E+03 3.50446555E+01
 4
 IC4H6OOH-I L 2/00C 4H 70 2 OG 300.000 5000.000
 1398.000 31
 1.73601429E+01 1.42046196E-02-4.65348263E-06 7.02209785E-10-3.99552775E-14 2
 -1.07509366E+03-6.12822377E+01 6.06669321E+00 3.94950065E-02-2.52721718E-05 3
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7.37319036E+03-9.55902415E+01-2.21863377E+00 8.91652629E-02-6.33360636E-
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4
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 4
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 HHC 3 P 4
 C5H1105r_3 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
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 04 3
 1.65633019E-07-5.83997145E-11-4.53560291E+04 2.73870555E+01
 4
 C5H1002_8 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
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 -3.85897387E+04-3.29661771E+01 1.45605273E+01-3.84482967E-02 2.23386053E-
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 05 3
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 C5H1104r_16 C 5 O 4 H 11 G 3E+02 1E+03 6E+02
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 1.16933102E-07-3.67838802E-11-4.86565479E+04 2.33976235E+01
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 04 3
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 0.76228585E+01 0.36928706E-01-0.18374225E-04 0.44953188E-08-0.43816239E-
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 05 3
 -0.27240453E-07 0.13184832E-10-0.36204795E+04 0.85539255E+01
 HHC 4 P 4
 C4H6O_Olef_5 C 4 O 1 H 6 G 3E+02 1E+03 6E+02
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 -4.31562560E-09 8.66884600E-12-1.05899350E+04 3.23228275E+01 4
 C5H8O4_Olef_2 C 5 O 4 H 8 G 3E+02 1E+03 6E+02
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 -5.24478531E+04 3.94348293E+01-2.13151289E+00 1.05852071E-01-1.22030176E-04 3
 7.30939229E-08-1.84812017E-11-5.24478531E+04 3.94348293E+01 4
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 3.95700219E-01 8.59909229E-02-9.64965596E-05 6.05181371E-08-1.54971353E-11 2
 -4.66489117E+04 2.46335087E+01 3.95700219E-01 8.59909229E-02-9.64965596E-05 3
 6.05181371E-08-1.54971353E-11-4.66489117E+04 2.46335087E+01 4
 C5H10O3_13 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 2.54586254E+01-1.08532298E-01 4.06902483E-04-4.75672899E-07 1.89533433E-10 2
 -6.81664310E+04-7.92708263E+01 2.54586254E+01-1.08532298E-01 4.06902483E-04 3
 -4.75672899E-07 1.89533433E-10-6.81664310E+04-7.92708263E+01 4
 Isoprenol H 10C 5O 1 0g 300.000 2500.0001000.000
 1
 0.56064701E+01 0.42822160E-01-0.21424503E-04 0.52579319E-08-0.51299617E-12 2
 -0.26095523E+05 0.11146029E+01 0.36207755E+01 0.34940835E-01 0.19536899E-04 3
 -0.46535213E-07 0.20189690E-10-0.25015219E+05 0.14320628E+02
 HHC 4 P 4
 CC(C)CCJ(*O) C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 3.01265319E+00 4.61458609E-02-1.99873473E-05-3.75183418E-09 4.58555202E-12 2
 -1.21024479E+04 1.37355200E+01 3.01265319E+00 4.61458609E-02-1.99873473E-05 3
 -3.75183418E-09 4.58555202E-12-1.21024479E+04 1.37355200E+01 4
 C5H11O3r_40 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 -8.22623306E-01 1.00136724E-01-1.24715574E-04 9.25525829E-08-2.90191464E-11 2
 -3.63763391E+04 2.92438192E+01-8.22623306E-01 1.00136724E-01-1.24715574E-04 3
 9.25525829E-08-2.90191464E-11-3.63763391E+04 2.92438192E+01 4
 C4H9O2r C 4 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 -1.16879015E+00 8.49349801E-02-1.10896157E-04 8.58093569E-08-2.80475020E-11 2

-6.20550376E+03 2.97182176E+01-1.16879015E+00 8.49349801E-02-1.10896157E-
 04 3
 8.58093569E-08-2.80475020E-11-6.20550376E+03 2.97182176E+01
 4
 C5H1104r_6 C 5 O 4 H 11 G 3E+02 1E+03 6E+02
 1
 -1.18542686E+00 1.22307779E-01-1.63775714E-04 1.20942387E-07-3.67838729E-
 11 2
 -5.18380323E+04 3.30609758E+01-1.18542686E+00 1.22307779E-01-1.63775714E-
 04 3
 1.20942387E-07-3.67838729E-11-5.18380323E+04 3.30609758E+01
 4
 C5H1103r_15 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 2.37606242E+00 7.09205582E-02-5.37651806E-05 2.47453453E-08-6.03086985E-
 12 2
 -2.93587105E+04 2.29870301E+01 2.37606242E+00 7.09205582E-02-5.37651806E-
 05 3
 2.47453453E-08-6.03086985E-12-2.93587105E+04 2.29870301E+01
 4
 C5H1002_1 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 2.63729332E+01-1.24488165E-01 4.34307478E-04-4.95970321E-07 1.95111156E-
 10 2
 -4.75101864E+04-8.47885753E+01 2.63729332E+01-1.24488165E-01 4.34307478E-
 04 3
 -4.95970321E-07 1.95111156E-10-4.75101864E+04-8.47885753E+01
 4
 C*CCC*O C 4 O 1 H 6 G 3E+02 1E+03 6E+02
 1
 2.57582511E+00 2.75311949E-02 5.49507059E-06-2.51098387E-08 1.17016848E-
 11 2
 -1.11357117E+04 1.74422749E+01 2.57582511E+00 2.75311949E-02 5.49507059E-
 06 3
 -2.51098387E-08 1.17016848E-11-1.11357117E+04 1.74422749E+01
 4
 C5H1003_3 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 -4.20308888E+00 1.09288444E-01-1.38253446E-04 1.03439526E-07-3.29310358E-
 11 2
 -4.20402542E+04 4.99257694E+01-4.20308888E+00 1.09288444E-01-1.38253446E-
 04 3
 1.03439526E-07-3.29310358E-11-4.20402542E+04 4.99257694E+01
 4
 C5H9O5r_Olef_18 C 5 O 5 H 9 G 3E+02 1E+03 6E+02
 1
 1.23345265E+01 4.34709627E-02-7.44951993E-06-1.97740047E-08 1.06545335E-
 11 2
 -3.59100443E+04-2.29296066E+01 1.23345265E+01 4.34709627E-02-7.44951993E-
 06 3
 -1.97740047E-08 1.06545335E-11-3.59100443E+04-2.29296066E+01
 4
 C*C(COOH)CCOH C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 1.04919939E+00 9.56801890E-02-1.29567880E-04 1.05579476E-07-3.57428686E-
 11 2
 -3.50780709E+04 2.51603601E+01 1.04919939E+00 9.56801890E-02-1.29567880E-
 04 3

1.05579476E-07-3.57428686E-11-3.50780709E+04 2.51603601E+01
 4
 C5H10O2_13 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 9.84172437E+00 1.22796060E-02 7.82955323E-05-1.08450105E-07 4.30842994E-
 11 2
 -4.05472183E+04-1.65700007E+01 9.84172437E+00 1.22796060E-02 7.82955323E-
 05 3
 -1.08450105E-07 4.30842994E-11-4.05472183E+04-1.65700007E+01
 4
 C*C(COJ)CCOH C 5 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 5.23909811E+00 5.09721358E-02-4.00730467E-05 2.39152551E-08-7.45427133E-
 12 2
 -1.73479644E+04 8.07928846E+00 5.23909811E+00 5.09721358E-02-4.00730467E-
 05 3
 2.39152551E-08-7.45427133E-12-1.73479644E+04 8.07928846E+00
 4
 C5H9O3r_8 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 3.00827772E+00 6.15268476E-02-3.47193399E-05 3.02013153E-09 3.25893157E-
 12 2
 -5.76909201E+04 1.45514043E+01 3.00827772E+00 6.15268476E-02-3.47193399E-
 05 3
 3.02013153E-09 3.25893157E-12-5.76909201E+04 1.45514043E+01
 4
 C5H10O2_olef C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 -6.11335949E+00 1.28773508E-01-1.88906535E-04 1.45285159E-07-4.40194990E-
 11 2
 -4.82687795E+04 4.94638689E+01-6.11335949E+00 1.28773508E-01-1.88906535E-
 04 3
 1.45285159E-07-4.40194990E-11-4.82687795E+04 4.94638689E+01
 4
 C5H11O5r_42 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 6.86254964E-01 1.20873304E-01-1.77781446E-04 1.53517445E-07-5.40647776E-
 11 2
 -4.41659756E+04 2.94999203E+01 6.86254964E-01 1.20873304E-01-1.77781446E-
 04 3
 1.53517445E-07-5.40647776E-11-4.41659756E+04 2.94999203E+01
 4
 C5H9O2r_2 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 3.77652377E+00 4.95249867E-02-1.78990916E-05-9.41848356E-09 7.02576217E-
 12 2
 -2.57865680E+04 1.02945103E+01 3.77652377E+00 4.95249867E-02-1.78990916E-
 05 3
 -9.41848356E-09 7.02576217E-12-2.57865680E+04 1.02945103E+01
 4
 C5H10O2_18 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 2.32748359E+01-8.85978221E-02 3.22567553E-04-3.57866029E-07 1.34863407E-
 10 2
 -4.58210840E+04-7.20641094E+01 2.32748359E+01-8.85978221E-02 3.22567553E-
 04 3
 -3.57866029E-07 1.34863407E-10-4.58210840E+04-7.20641094E+01
 4

C5H9O3r_Olef C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.60167620E+01-1.62261107E-02 1.24329232E-04-1.46202146E-07 5.56474224E-
 11 2
 -2.42217363E+04-3.73125944E+01 1.60167620E+01-1.62261107E-02 1.24329232E-
 04 3
 -1.46202146E-07 5.56474224E-11-2.42217363E+04-3.73125944E+01
 4
 C5H10O3_12 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 2.25366614E+01-6.92167672E-02 2.83731260E-04-3.25453033E-07 1.24950747E-
 10 2
 -6.76673821E+04-6.86592253E+01 2.25366614E+01-6.92167672E-02 2.83731260E-
 04 3
 -3.25453033E-07 1.24950747E-10-6.76673821E+04-6.86592253E+01
 4
 C5H10O3_2 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 2.26126576E+00 7.74081220E-02-7.75192977E-05 5.04163033E-08-1.54947497E-
 11 2
 -4.41747553E+04 1.92139944E+01 2.26126576E+00 7.74081220E-02-7.75192977E-
 05 3
 5.04163033E-08-1.54947497E-11-4.41747553E+04 1.92139944E+01
 4
 C4H9O4r C 4 O 4 H 9 G 3E+02 1E+03 6E+02
 1
 -3.25358985E+00 1.28496304E-01-2.07800625E-04 1.80761347E-07-6.26098116E-
 11 2
 -1.89081972E+04 3.93462451E+01-3.25358985E+00 1.28496304E-01-2.07800625E-
 04 3
 1.80761347E-07-6.26098116E-11-1.89081972E+04 3.93462451E+01
 4
 C5H10O4_15 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
 1
 1.22532237E+00 9.70316424E-02-1.09293843E-04 6.96948241E-08-1.91240354E-
 11 2
 -6.40844317E+04 2.39487648E+01 1.22532237E+00 9.70316424E-02-1.09293843E-
 04 3
 6.96948241E-08-1.91240354E-11-6.40844317E+04 2.39487648E+01
 4
 C5H11O5r_6 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 6.86254964E-01 1.20873304E-01-1.77781446E-04 1.53517445E-07-5.40647776E-
 11 2
 -4.41659756E+04 2.94999203E+01 6.86254964E-01 1.20873304E-01-1.77781446E-
 04 3
 1.53517445E-07-5.40647776E-11-4.41659756E+04 2.94999203E+01
 4
 C5H8O2_Olef_1 C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1
 4.07328751E+00 4.59698421E-02-1.88685187E-05-5.55237355E-09 5.28835769E-
 12 2
 -3.76037834E+04 1.07462930E+01 4.07328751E+00 4.59698421E-02-1.88685187E-
 05 3
 -5.55237355E-09 5.28835769E-12-3.76037834E+04 1.07462930E+01
 4
 C5H11O3r_28 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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1.81064843E+01-3.22348147E-02 1.83856060E-04-2.12586103E-07 8.04079367E-
 11 2
 -3.45398021E+04-4.41085358E+01 1.81064843E+01-3.22348147E-02 1.83856060E-
 04 3
 -2.12586103E-07 8.04079367E-11-3.45398021E+04-4.41085358E+01
 4
 C*(C)CCJ(*O) C 5 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 6.58924766E-01 5.92430419E-02-6.27629435E-05 4.04331155E-08-1.11877602E-
 11 2
 3.33309754E+03 2.46728994E+01 6.58924766E-01 5.92430419E-02-6.27629435E-
 05 3
 4.04331155E-08-1.11877602E-11 3.33309754E+03 2.46728994E+01
 4
 C5H8O3_Olef C 5 O 3 H 8 G 3E+02 1E+03 6E+02
 1
 -4.52454973E+00 1.37447100E-01-2.41527187E-04 2.22644059E-07-7.90107985E-
 11 2
 -2.93176628E+04 4.36862484E+01-4.52454973E+00 1.37447100E-01-2.41527187E-
 04 3
 2.22644059E-07-7.90107985E-11-2.93176628E+04 4.36862484E+01
 4
 C4H5Or_Olef C 4 O 1 H 5 G 3E+02 1E+03 6E+02
 1
 2.55174657E+00 2.99989604E-02-8.60794224E-06-8.63550984E-09 5.41943917E-
 12 2
 1.52941031E+04 1.51332259E+01 2.55174657E+00 2.99989604E-02-8.60794224E-
 06 3
 -8.63550984E-09 5.41943917E-12 1.52941031E+04 1.51332259E+01
 4
 CC(C)CJCOH C 5 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 2.40328782E+00 5.25153678E-02-1.76071528E-05-1.25707130E-08 8.92908180E-
 12 2
 -1.65658352E+04 1.79884629E+01 2.40328782E+00 5.25153678E-02-1.76071528E-
 05 3
 -1.25707130E-08 8.92908180E-12-1.65658352E+04 1.79884629E+01
 4
 C5H9Or_Olef_1 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 -3.09567514E+00 9.05363175E-02-1.09635774E-04 7.22941535E-08-1.93158526E-
 11 2
 -1.75503730E+03 3.70024875E+01-3.09567514E+00 9.05363175E-02-1.09635774E-
 04 3
 7.22941535E-08-1.93158526E-11-1.75503730E+03 3.70024875E+01
 4
 C4H6O_Olef_4 C 4 O 1 H 6 G 3E+02 1E+03 6E+02
 1
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 11 2
 -9.26965667E+03 4.60822795E+01-5.17940398E+00 8.11199405E-02-9.69327011E-
 05 3
 5.76450244E-08-1.32355164E-11-9.26965667E+03 4.60822795E+01
 4
 C5H9O3r_11 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.55838870E+01-1.96933492E-02 1.33693730E-04-1.45028752E-07 5.12192845E-
 11 2

-4.64611740E+04-2.57026510E+01 1.55838870E+01-1.96933492E-02 1.33693730E-
 04 3
 -1.45028752E-07 5.12192845E-11-4.64611740E+04-2.57026510E+01
 4
 C5H11O5r_20 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 3.56536110E+00 1.01742461E-01-1.35614452E-04 1.17881430E-07-4.35869495E-
 11 2
 -3.55976113E+04 1.75661167E+01 3.56536110E+00 1.01742461E-01-1.35614452E-
 04 3
 1.17881430E-07-4.35869495E-11-3.55976113E+04 1.75661167E+01
 4
 C5H8O4_Olef_4 C 5 O 4 H 8 G 3E+02 1E+03 6E+02
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 -5.03846742E+00 1.53393490E-01-2.68078141E-04 2.44650417E-07-8.61544272E-
 11 2
 -6.04072768E+04 4.64091706E+01-5.03846742E+00 1.53393490E-01-2.68078141E-
 04 3
 2.44650417E-07-8.61544272E-11-6.04072768E+04 4.64091706E+01
 4
 C5H9O3r_4 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 8.07740865E+00 3.73492642E-02 7.20883372E-06-3.45881431E-08 1.65716846E-
 11 2
 -4.27215119E+04-3.04918931E+00 8.07740865E+00 3.73492642E-02 7.20883372E-
 06 3
 -3.45881431E-08 1.65716846E-11-4.27215119E+04-3.04918931E+00
 4
 C5H8O_Olef_1 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 -4.01697496E+00 9.52572695E-02-1.35478400E-04 1.05686747E-07-3.29028017E-
 11 2
 -1.39945316E+04 4.17665683E+01-4.01697496E+00 9.52572695E-02-1.35478400E-
 04 3
 1.05686747E-07-3.29028017E-11-1.39945316E+04 4.17665683E+01
 4
 C5H11O5r_18 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 1.76852212E+00 1.13154833E-01-1.57533750E-04 1.34874994E-07-4.83452887E-
 11 2
 -3.80541398E+04 2.22520798E+01 1.76852212E+00 1.13154833E-01-1.57533750E-
 04 3
 1.34874994E-07-4.83452887E-11-3.80541398E+04 2.22520798E+01
 4
 C2H2O3 C 2 O 3 H 2 G 3E+02 1E+03 6E+02
 1
 2.47426750E+00 2.80757953E-02-2.44034640E-05 1.34011876E-08-3.56304521E-
 12 2
 -5.85050025E+04 1.41942808E+01 2.47426750E+00 2.80757953E-02-2.44034640E-
 05 3
 1.34011876E-08-3.56304521E-12-5.85050025E+04 1.41942808E+01
 4
 C5H11O3r_23 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 -4.47252367E-01 1.02926724E-01-1.24939422E-04 8.85293907E-08-2.68712133E-
 11 2
 -2.99917342E+04 2.96560916E+01-4.47252367E-01 1.02926724E-01-1.24939422E-
 04 3

8.85293907E-08-2.68712133E-11-2.99917342E+04 2.96560916E+01
 4
 C5H11O3r_16 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -3.39198106E+04 2.45578561E+01 9.74215681E-01 8.87243519E-02-1.02796276E-
 04 3
 7.55590188E-08-2.42608072E-11-3.39198106E+04 2.45578561E+01
 4
 C*C(C*O)CCOH C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1
 3.37097525E+00 4.48702537E-02-9.98591739E-06-1.74802519E-08 1.01596611E-
 11 2
 -3.68843961E+04 1.59495039E+01 3.37097525E+00 4.48702537E-02-9.98591739E-
 06 3
 -1.74802519E-08 1.01596611E-11-3.68843961E+04 1.59495039E+01
 4
 C4H6O3 C 4 O 3 H 6 G 3E+02 1E+03 6E+02
 1
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 11 2
 -5.84843231E+04-3.58238926E+00 8.09736446E+00 1.77244883E-02 3.00089011E-
 05 3
 -4.76611202E-08 1.89666310E-11-5.84843231E+04-3.58238926E+00
 4
 C5H11O3r C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 4.34903471E+00 6.29333736E-02-4.32771797E-05 1.98673555E-08-5.60746751E-
 12 2
 -2.80922356E+04 1.68813493E+01 4.34903471E+00 6.29333736E-02-4.32771797E-
 05 3
 1.98673555E-08-5.60746751E-12-2.80922356E+04 1.68813493E+01
 4
 C2H5O2r C 2 O 2 H 5 G 3E+02 1E+03 6E+02
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 13 2
 8.86659452E+02 1.91617699E+01 1.42309384E+00 3.76503602E-02-3.07596359E-
 05 3
 9.66464525E-09 2.64406635E-13 8.86659452E+02 1.91617699E+01
 4
 C5H6O2_Olef_1 C 5 O 2 H 6 G 3E+02 1E+03 6E+02
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 -3.11239879E+04 3.44753923E+01-2.20277387E+00 8.66371642E-02-1.21945224E-
 04 3
 9.95843313E-08-3.31082687E-11-3.11239879E+04 3.44753923E+01
 4
 C5H11O5r_10 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 8.62388269E-01 1.24298491E-01-1.89212744E-04 1.65633019E-07-5.83997145E-
 11 2
 -4.68154477E+04 2.73870555E+01 8.62388269E-01 1.24298491E-01-1.89212744E-
 04 3
 1.65633019E-07-5.83997145E-11-4.68154477E+04 2.73870555E+01
 4

C5H9O3r C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 2.80892891E+01-1.04824143E-01 3.27313360E-04-3.38043134E-07 1.21515965E-
 10 2
 -4.98358659E+04-8.64849316E+01 2.80892891E+01-1.04824143E-01 3.27313360E-
 04 3
 -3.38043134E-07 1.21515965E-10-4.98358659E+04-8.64849316E+01
 4
 C5H8O2_Olef_13 C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1
 2.13138626E+01-6.85479227E-02 2.60058756E-04-2.93857128E-07 1.12138547E-
 10 2
 -3.11012335E+04-6.68866628E+01 2.13138626E+01-6.85479227E-02 2.60058756E-
 04 3
 -2.93857128E-07 1.12138547E-10-3.11012335E+04-6.68866628E+01
 4
 C4H8O4 C 4 O 4 H 8 G 3E+02 1E+03 6E+02
 1
 -1.99314753E+00 9.72320330E-02-1.31143333E-04 1.02658168E-07-3.35762357E-
 11 2
 -6.12958096E+04 4.17663192E+01-1.99314753E+00 9.72320330E-02-1.31143333E-
 04 3
 1.02658168E-07-3.35762357E-11-6.12958096E+04 4.17663192E+01
 4
 C5H10O2_7 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 1.25875550E+01-3.04611121E-02 2.12898052E-04-2.70785546E-07 1.12001923E-
 10 2
 -3.98562136E+04-2.50687369E+01 1.25875550E+01-3.04611121E-02 2.12898052E-
 04 3
 -2.70785546E-07 1.12001923E-10-3.98562136E+04-2.50687369E+01
 4
 C5H10O3_Olef_5 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 1.75151165E+00 9.67797774E-02-1.38450481E-04 1.17507354E-07-4.06141721E-
 11 2
 -3.57974582E+04 1.99571491E+01 1.75151165E+00 9.67797774E-02-1.38450481E-
 04 3
 1.17507354E-07-4.06141721E-11-3.57974582E+04 1.99571491E+01
 4
 C5H10O2_4 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 2.32340723E+01-1.05984864E-01 3.80527460E-04-4.24671257E-07 1.61289036E-
 10 2
 -5.47204607E+04-6.99192649E+01 2.32340723E+01-1.05984864E-01 3.80527460E-
 04 3
 -4.24671257E-07 1.61289036E-10-5.47204607E+04-6.99192649E+01
 4
 C5H10O4_5 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
 1
 1.61243159E+00 9.85244318E-02-1.22843099E-04 9.09607069E-08-2.87195213E-
 11 2
 -6.21741064E+04 2.31283631E+01 1.61243159E+00 9.85244318E-02-1.22843099E-
 04 3
 9.09607069E-08-2.87195213E-11-6.21741064E+04 2.31283631E+01
 4
 C2H5O3r C 2 O 3 H 5 G 3E+02 1E+03 6E+02
 1

4.76651628E-01 6.65327790E-02-1.09521094E-04 9.67328707E-08-3.37626334E-
11 2
-1.87615467E+04 2.48885062E+01 4.76651628E-01 6.65327790E-02-1.09521094E-
04 3
9.67328707E-08-3.37626334E-11-1.87615467E+04 2.48885062E+01
4
C5H9O5r_Olef_3 C 5 O 5 H 9 G 3E+02 1E+03 6E+02
1
-4.48912138E+00 1.55265066E-01-2.52352475E-04 2.12664438E-07-7.12226124E-
11 2
-3.23361809E+04 4.86229485E+01-4.48912138E+00 1.55265066E-01-2.52352475E-
04 3
2.12664438E-07-7.12226124E-11-3.23361809E+04 4.86229485E+01
4
C5H11O5r_32 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
1
2.17295797E+01-2.74874880E-02 1.64857301E-04-1.78552039E-07 6.26060369E-
11 2
-4.23163162E+04-6.04989527E+01 2.17295797E+01-2.74874880E-02 1.64857301E-
04 3
-1.78552039E-07 6.26060369E-11-4.23163162E+04-6.04989527E+01
4
C5H10O2_21 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
1.07907160E+01-1.90487399E-02 1.90978754E-04-2.53791981E-07 1.07243583E-
10 2
-4.23127420E+04-1.92841615E+01 1.07907160E+01-1.90487399E-02 1.90978754E-
04 3
-2.53791981E-07 1.07243583E-10-4.23127420E+04-1.92841615E+01
4
C5H9O2r_Olef_4 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
1
3.23897373E+00 6.54631389E-02-6.50699026E-05 4.13929106E-08-1.18581881E-
11 2
-1.97752005E+04 1.26769681E+01 3.23897373E+00 6.54631389E-02-6.50699026E-
05 3
4.13929106E-08-1.18581881E-11-1.97752005E+04 1.26769681E+01
4
C5H11O3r_10 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
1
1.52571993E+00 9.49395395E-02-1.14451421E-04 8.36514010E-08-2.64478110E-
11 2
-2.87252593E+04 2.28572636E+01 1.52571993E+00 9.49395395E-02-1.14451421E-
04 3
8.36514010E-08-2.64478110E-11-2.87252593E+04 2.28572636E+01
4
C5H9Or_Olef_4 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
1.94948280E+00 6.22531262E-02-5.35105444E-05 2.30066386E-08-3.13569587E-
12 2
-2.12312503E+03 1.82154040E+01 1.94948280E+00 6.22531262E-02-5.35105444E-
05 3
2.30066386E-08-3.13569587E-12-2.12312503E+03 1.82154040E+01
4
CC(C)(C)CJCOH C 6 O 1 H 13 G 3E+02 1E+03 6E+02
1
1.16264113E+00 6.95459131E-02-3.00618944E-05-1.08861946E-08 1.03083343E-
11 2

-2.07073739E+04 1.94541569E+01 1.16264113E+00 6.95459131E-02-3.00618944E-
 05 3
 -1.08861946E-08 1.03083343E-11-2.07073739E+04 1.94541569E+01
 4
 C*C(COOJ)CCOH C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.01336675E+00 9.42832482E-02-1.40308217E-04 1.22090264E-07-4.25817495E-
 11 2
 -1.67727239E+04 2.62362354E+01 1.01336675E+00 9.42832482E-02-1.40308217E-
 04 3
 1.22090264E-07-4.25817495E-11-1.67727239E+04 2.62362354E+01
 4
 C5H1103r_9 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 2.11532711E+00 8.46643197E-02-9.25923229E-05 6.53877131E-08-2.08748886E-
 11 2
 -2.68120001E+04 2.29305272E+01 2.11532711E+00 8.46643197E-02-9.25923229E-
 05 3
 6.53877131E-08-2.08748886E-11-2.68120001E+04 2.29305272E+01
 4
 C5H8O2_Olef_8 C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1
 -2.21041186E+00 9.50850524E-02-1.02243384E-04 5.08282720E-08-8.68580451E-
 12 2
 -4.04926285E+04 1.63353707E+01-2.21041186E+00 9.50850524E-02-1.02243384E-
 04 3
 5.08282720E-08-8.68580451E-12-4.04926285E+04 1.63353707E+01
 4
 C5H1105r_29 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 1.44716331E+01 2.68462509E-02 4.36279795E-05-7.16673308E-08 2.90444557E-
 11 2
 -5.32793670E+04-3.13185304E+01 1.44716331E+01 2.68462509E-02 4.36279795E-
 05 3
 -7.16673308E-08 2.90444557E-11-5.32793670E+04-3.13185304E+01
 4
 C4H6O_Olef C 4 O 1 H 6 G 3E+02 1E+03 6E+02
 1
 3.31569670E+00 2.86599859E-02-2.48637831E-06-1.41107077E-08 6.92009504E-
 12 2
 -4.88155786E+00 1.32769845E+01 3.31569670E+00 2.86599859E-02-2.48637831E-
 06 3
 -1.41107077E-08 6.92009504E-12-4.88155786E+00 1.32769845E+01
 4
 C4H8O_Olef_1 C 4 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 3.72222522E+00 3.51450938E-02-1.04987176E-05-7.98601495E-09 5.29708428E-
 12 2
 -2.18758738E+04 1.01985353E+01 3.72222522E+00 3.51450938E-02-1.04987176E-
 05 3
 -7.98601495E-09 5.29708428E-12-2.18758738E+04 1.01985353E+01
 4
 C4H7O3r_1 C 4 O 3 H 7 G 3E+02 1E+03 6E+02
 1
 2.19675119E+00 5.25239797E-02-4.16484996E-05 2.09939475E-08-5.28763843E-
 12 2
 -4.35657031E+04 2.35866353E+01 2.19675119E+00 5.25239797E-02-4.16484996E-
 05 3

2.09939475E-08-5.28763843E-12-4.35657031E+04 2.35866353E+01
4
CCJ(C)CCOH C 5 O 1 H 11 G 3E+02 1E+03 6E+02
1
4.78520015E+00 3.30684739E-02 2.60005073E-05-5.32441788E-08 2.27677369E-
11 2
-1.78297178E+04 9.65498580E+00 4.78520015E+00 3.30684739E-02 2.60005073E-
05 3
-5.32441788E-08 2.27677369E-11-1.78297178E+04 9.65498580E+00
4
C5H10O2_25 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
7.86875208E+00 2.02667906E-02 6.78075314E-05-1.03572115E-07 4.26608971E-
11 2
-4.18136932E+04-8.67256042E+00 7.86875208E+00 2.02667906E-02 6.78075314E-
05 3
-1.03572115E-07 4.26608971E-11-4.18136932E+04-8.67256042E+00
4
C5H10O2_2 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
7.86875208E+00 2.02667906E-02 6.78075314E-05-1.03572115E-07 4.26608971E-
11 2
-4.18136932E+04-8.67256042E+00 7.86875208E+00 2.02667906E-02 6.78075314E-
05 3
-1.03572115E-07 4.26608971E-11-4.18136932E+04-8.67256042E+00
4
C5H11Or_1 C 5 O 1 H 11 G 3E+02 1E+03 6E+02
1
3.70809983E+00 5.04311741E-02-1.52672674E-05-1.46162772E-08 9.72693992E-
12 2
-1.53876482E+04 1.04411759E+01 3.70809983E+00 5.04311741E-02-1.52672674E-
05 3
-1.46162772E-08 9.72693992E-12-1.53876482E+04 1.04411759E+01
4
C4H6O3_1 C 4 O 3 H 6 G 3E+02 1E+03 6E+02
1
4.63307673E-01 4.76341138E-02-1.56653957E-05-1.24114177E-08 8.10041402E-
12 2
-7.13870250E+04 2.88051083E+01 4.63307673E-01 4.76341138E-02-1.56653957E-
05 3
-1.24114177E-08 8.10041402E-12-7.13870250E+04 2.88051083E+01
4
C5H10O4 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
1
1.93444166E+01-2.83383819E-02 1.70187497E-04-1.97245795E-07 7.44785517E-
11 2
-6.73111869E+04-4.89457642E+01 1.93444166E+01-2.83383819E-02 1.70187497E-
04 3
-1.97245795E-07 7.44785517E-11-6.73111869E+04-4.89457642E+01
4
C5H11O3r_36 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
1
3.18488120E-01 9.60766919E-02-1.14511621E-04 8.23812771E-08-2.56332278E-
11 2
-2.92685286E+04 2.76164903E+01 3.18488120E-01 9.60766919E-02-1.14511621E-
04 3
8.23812771E-08-2.56332278E-11-2.92685286E+04 2.76164903E+01
4

C5H11O3r_2 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 1.76159621E+00 9.80326157E-02-1.26147014E-04 9.66356800E-08-3.12061575E-
 11 2
 -2.80003034E+04 1.78798746E+01 1.76159621E+00 9.80326157E-02-1.26147014E-
 04 3
 9.66356800E-08-3.12061575E-11-2.80003034E+04 1.78798746E+01
 4
 CCJ*CCOH C 4 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 4.65193297E+00 3.16825226E-02-1.20490197E-05-3.77581145E-09 3.41755442E-
 12 2
 6.38090331E+03 5.83156990E+00 4.65193297E+00 3.16825226E-02-1.20490197E-
 05 3
 -3.77581145E-09 3.41755442E-12 6.38090331E+03 5.83156990E+00
 4
 C5H11O3r_25 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 1.57245719E+01-1.27879208E-02 1.40248400E-04-1.71912637E-07 6.65692816E-
 11 2
 -3.32759194E+04-3.57750587E+01 1.57245719E+01-1.27879208E-02 1.40248400E-
 04 3
 -1.71912637E-07 6.65692816E-11-3.32759194E+04-3.57750587E+01
 4
 C5H11O3r_39 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 1.15034899E+00 9.21495395E-02-1.14227573E-04 8.76745931E-08-2.85957441E-
 11 2
 -3.51098642E+04 2.24449912E+01 1.15034899E+00 9.21495395E-02-1.14227573E-
 04 3
 8.76745931E-08-2.85957441E-11-3.51098642E+04 2.24449912E+01
 4
 CC(C)*CC C 5 H 10 G 3E+02 1E+03 6E+02
 1
 2.29238000E+00 3.69500000E-02-1.72999997E-06-1.34800000E-08 5.13200000E-
 12 2
 -7.15700000E+03 1.66600000E+01 2.29238000E+00 3.69500000E-02-1.72999997E-
 06 3
 -1.34800000E-08 5.13200000E-12-7.15700000E+03 1.66600000E+01
 4
 CC(C)C*C C 5 H 10 G 3E+02 1E+03 6E+02
 1
 4.64685999E-01 5.22600000E-02-3.04100000E-05 7.71399999E-09-3.78899999E-
 13 2
 -5.51500000E+03 2.35600000E+01 4.64685999E-01 5.22600000E-02-3.04100000E-
 05 3
 7.71399999E-09-3.78899999E-13-5.51500000E+03 2.35600000E+01
 4
 C5H10O_Olef C 5 O 1 H 10 G 3E+02 1E+03 6E+02
 1
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 11 2
 -2.69973829E+04 3.44141180E+01-2.24700995E+00 8.45008388E-02-9.12858350E-
 05 3
 5.54162785E-08-1.39003369E-11-2.69973829E+04 3.44141180E+01
 4
 C5H8O2_Olef_5 C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1

1.19555805E+00 7.16869026E-02-6.51919426E-05 2.82102433E-08-3.82798643E-
 12 2
 -2.62571820E+04 1.55506710E+01 1.19555805E+00 7.16869026E-02-6.51919426E-
 05 3
 2.82102433E-08-3.82798643E-12-2.62571820E+04 1.55506710E+01
 4
 C4H5O2r_Olef C 4 O 2 H 5 G 3E+02 1E+03 6E+02
 1
 -2.13804609E+00 8.82962348E-02-1.41676680E-04 1.23367252E-07-4.21227008E-
 11 2
 -1.82289153E+04 3.22835914E+01-2.13804609E+00 8.82962348E-02-1.41676680E-
 04 3
 1.23367252E-07-4.21227008E-11-1.82289153E+04 3.22835914E+01
 4
 C5H9O5r_Olef_9 C 5 O 5 H 9 G 3E+02 1E+03 6E+02
 1
 -4.48912138E+00 1.55265066E-01-2.52352475E-04 2.12664438E-07-7.12226124E-
 11 2
 -3.23361809E+04 4.86229485E+01-4.48912138E+00 1.55265066E-01-2.52352475E-
 04 3
 2.12664438E-07-7.12226124E-11-3.23361809E+04 4.86229485E+01
 4
 C5H10O4_10 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
 1
 -4.97133493E+00 1.21290305E-01-1.55073695E-04 1.15878141E-07-3.66978664E-
 11 2
 -7.39446064E+04 5.41826634E+01-4.97133493E+00 1.21290305E-01-1.55073695E-
 04 3
 1.15878141E-07-3.66978664E-11-7.39446064E+04 5.41826634E+01
 4
 C5H9Or C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 4.78318397E+00 3.42928158E-02 1.07006710E-05-3.53637790E-08 1.59890535E-
 11 2
 -6.14719237E+03 6.08882985E+00 4.78318397E+00 3.42928158E-02 1.07006710E-
 05 3
 -3.53637790E-08 1.59890535E-11-6.14719237E+03 6.08882985E+00
 4
 C5H11O3r_5 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 1.15034899E+00 9.21495395E-02-1.14227573E-04 8.76745931E-08-2.85957441E-
 11 2
 -3.65692827E+04 2.24449912E+01 1.15034899E+00 9.21495395E-02-1.14227573E-
 04 3
 8.76745931E-08-2.85957441E-11-3.65692827E+04 2.24449912E+01
 4
 C5H9O2r_Olef_3 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 5.94141037E+00 5.20717242E-02-4.89556480E-05 3.58431334E-08-1.23255748E-
 11 2
 -1.80673517E+04 1.77746518E+00 5.94141037E+00 5.20717242E-02-4.89556480E-
 05 3
 3.58431334E-08-1.23255748E-11-1.80673517E+04 1.77746518E+00
 4
 C5H9O3r_13 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 9.53796125E+00 2.29130160E-02 4.03908630E-05-6.28755481E-08 2.49184647E-
 11 2

-4.50274865E+04-8.69807290E+00 9.53796125E+00 2.29130160E-02 4.03908630E-05 3
 -6.28755481E-08 2.49184647E-11-4.50274865E+04-8.69807290E+00
 4
 C5H6O3_Olef C 5 O 3 H 6 G 3E+02 1E+03 6E+02
 1
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 -6.22136020E+04 3.71983144E+01-2.71669155E+00 1.02583554E-01-1.48496179E-04 3
 1.21590689E-07-4.02518975E-11-6.22136020E+04 3.71983144E+01
 4
 C5H9O2r_Olef_7 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
 1
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 -2.10970849E+04 3.20403745E+01-2.13440490E+00 9.63129782E-02-1.19655604E-04 3
 8.16822950E-08-2.27374625E-11-2.10970849E+04 3.20403745E+01
 4
 C5H11O5r_47 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
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 -1.11058402E+00 1.32285676E-01-1.99700744E-04 1.70511009E-07-5.88231168E-11 2
 -4.80819226E+04 3.41858835E+01-1.11058402E+00 1.32285676E-01-1.99700744E-04 3
 1.70511009E-07-5.88231168E-11-4.80819226E+04 3.41858835E+01
 4
 C5H11O3r_6 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 3.18488120E-01 9.60766919E-02-1.14511621E-04 8.23812771E-08-2.56332278E-11 2
 -2.92685286E+04 2.76164903E+01 3.18488120E-01 9.60766919E-02-1.14511621E-04 3
 8.23812771E-08-2.56332278E-11-2.92685286E+04 2.76164903E+01
 4
 C5H10O3_Olef_6 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
 1
 -2.77117765E+00 1.11455936E-01-1.34830242E-04 8.72031649E-08-2.37947594E-11 2
 -4.13804560E+04 3.99589896E+01-2.77117765E+00 1.11455936E-01-1.34830242E-04 3
 8.72031649E-08-2.37947594E-11-4.13804560E+04 3.99589896E+01
 4
 C5H11O3r_19 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 3.85332182E+00 6.95935087E-02-6.06292816E-05 3.99230043E-08-1.37829790E-11 2
 -2.53514464E+04 1.26240524E+01 3.85332182E+00 6.95935087E-02-6.06292816E-05 3
 3.99230043E-08-1.37829790E-11-2.53514464E+04 1.26240524E+01
 4
 C4H5Or_Olef_1 C 4 O 1 H 5 G 3E+02 1E+03 6E+02
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1.01360893E-07-3.49790720E-11 1.28606988E+04 2.95606692E+01
 4
 C5H9O2r C 5 O 2 H 9 G 3E+02 1E+03 6E+02
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 8.24800346E+00 2.12876966E-02 3.38948336E-05-4.82414813E-08 1.75521869E-
 11 2
 -2.39881204E+04-4.75026490E+00 8.24800346E+00 2.12876966E-02 3.38948336E-
 05 3
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 4
 C5H11O3r_37 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -2.89373393E+04 3.07392780E+01-9.41186639E-01 1.05171534E-01-1.30354095E-
 04 3
 9.30576218E-08-2.81124061E-11-2.89373393E+04 3.07392780E+01
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 C5H10O4_12 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
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 12 2
 -6.39364949E+04 1.29351287E+01 6.83901450E+00 5.67924121E-02-2.34321327E-
 05 3
 -4.23141261E-09 4.18187110E-12-6.39364949E+04 1.29351287E+01
 4
 CC(C)CCJOH C 5 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 1.81368064E+00 6.27905875E-02-3.94662509E-05 5.69297493E-09 3.35615943E-
 12 2
 -1.84790944E+04 1.79151993E+01 1.81368064E+00 6.27905875E-02-3.94662509E-
 05 3
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 4
 C5H10O2_23 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
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 11 2
 -5.07130698E+04-6.52771591E+00 7.82798852E+00 2.87974912E-03 1.25767439E-
 04 3
 -1.70377343E-07 6.90865264E-11-5.07130698E+04-6.52771591E+00
 4
 C5H11O3r_4 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -3.26533357E+04 1.77590281E+01 2.94718797E+00 8.07371673E-02-9.23082751E-
 05 3
 7.06810290E-08-2.38374049E-11-3.26533357E+04 1.77590281E+01
 4
 C5H10O3_Olef_2 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
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 11 2
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 04 3
 1.23057131E-07-4.01467854E-11-3.75053070E+04 3.08566520E+01
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C5H10O3_Olef_1 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
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 2
 -3.91251748E+04 5.56870122E+01-7.45998471E+00 1.52953777E-01-2.46974711E-04
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 2.07824153E-07-6.86691490E-11-3.91251748E+04 5.56870122E+01
 4
 C5H11O3r_26 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 1.65564328E+01-1.67150733E-02 1.40532448E-04-1.66619321E-07 6.36067654E-11
 2
 -3.91172550E+04-4.09465578E+01 1.65564328E+01-1.67150733E-02 1.40532448E-04
 3
 -1.66619321E-07 6.36067654E-11-3.91172550E+04-4.09465578E+01
 4
 C5H11O4r_7 C 5 O 4 H 11 G 3E+02 1E+03 6E+02
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 3.90229294E-01 1.12938036E-01-1.46976727E-04 1.07711676E-07-3.27745651E-11
 2
 -4.86477160E+04 2.62163281E+01 3.90229294E-01 1.12938036E-01-1.46976727E-04
 3
 1.07711676E-07-3.27745651E-11-4.86477160E+04 2.62163281E+01
 4
 C5H9O3r_Olef_13 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 2
 -2.29511003E+04 4.87368113E+01-5.39383703E+00 1.26672435E-01-1.68693941E-04
 3
 1.16382736E-07-3.29758379E-11-2.29511003E+04 4.87368113E+01
 4
 C5H8O2_Olef C 5 O 2 H 8 G 3E+02 1E+03 6E+02
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 2
 -5.11462049E+04 3.77224747E+01-3.35635631E+00 1.08187419E-01-1.61296245E-04
 3
 1.35699931E-07-4.55654551E-11-5.11462049E+04 3.77224747E+01
 4
 C5H10O_Olef_2 C 5 O 1 H 10 G 3E+02 1E+03 6E+02
 1
 4.21034399E-01 6.85771430E-02-5.77036565E-05 2.42749874E-08-3.19828317E-12
 2
 -2.77017571E+04 2.49781716E+01 4.21034399E-01 6.85771430E-02-5.77036565E-05
 3
 2.42749874E-08-3.19828317E-12-2.77017571E+04 2.49781716E+01
 4
 C4H9O3r C 4 O 3 H 9 G 3E+02 1E+03 6E+02
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 2
 -2.80518019E+04 3.31231018E+01-1.90696464E+00 1.04316035E-01-1.49732449E-04
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 1.18222353E-07-3.79601616E-11-2.80518019E+04 3.31231018E+01
 4
 C2H3O2r C 2 O 2 H 3 G 3E+02 1E+03 6E+02
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6.60813086E-01 3.36250473E-02-3.14882527E-05 1.67836398E-08-4.00508126E-
 12 2
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 05 3
 1.67836398E-08-4.00508126E-12-2.97450445E+04 2.21855408E+01
 4
 C5H10O2_Olef_3 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
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 12 2
 -4.96920079E+04 2.44331334E+01 3.84691078E-01 8.10357441E-02-8.00149212E-
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 4
 C4H6O2_Olef C 4 O 2 H 6 G 3E+02 1E+03 6E+02
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 04 3
 1.78132527E-07-6.05617739E-11-3.86763007E+04 5.08108265E+01
 4
 C4H6O2 C 4 O 2 H 6 G 3E+02 1E+03 6E+02
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 11 2
 -3.93743804E+04 1.70595676E+01 3.44883089E+00 2.89584207E-02 7.31651034E-
 06 3
 -2.82816246E-08 1.29535048E-11-3.93743804E+04 1.70595676E+01
 4
 C5H7O2r_Olef_1 C 5 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 -3.34651012E-01 9.27390463E-02-1.52032354E-04 1.40979838E-07-5.07222012E-
 11 2
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 1.40979838E-07-5.07222012E-11-1.15875563E+04 2.55065645E+01
 4
 C4H7O2r_3 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
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 4.93274877E+00 2.40438633E-02 2.31943236E-05-4.29529056E-08 1.76175650E-
 11 2
 -3.55259907E+04 8.76450327E+00 4.93274877E+00 2.40438633E-02 2.31943236E-
 05 3
 -4.29529056E-08 1.76175650E-11-3.55259907E+04 8.76450327E+00
 4
 C5H11O3r_7 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 04 3
 1.00644965E-07-3.12061502E-11-3.11817878E+04 2.75432268E+01
 4
 C5H10O4_7 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
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 4.58613544E-08-1.45032410E-11-7.36225790E+04 1.76863130E+01
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 C5H11O3r_48 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -2.79914714E+04 2.06985791E+01 1.30453709E+00 9.69821688E-02-1.19571732E-
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 8.74142539E-08-2.71968424E-11-2.79914714E+04 2.06985791E+01
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 CCJ(C)CC*O C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 C5H11O5r_9 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -4.66225040E+04 3.41858835E+01-1.11058402E+00 1.32285676E-01-1.99700744E-
 04 3
 1.70511009E-07-5.88231168E-11-4.66225040E+04 3.41858835E+01
 4
 C5H9Or_2 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 1.10177922E+00 5.06075731E-02-1.45301028E-05-1.68630054E-08 1.06870685E-
 11 2
 -1.16239667E+04 2.14697651E+01 1.10177922E+00 5.06075731E-02-1.45301028E-
 05 3
 -1.68630054E-08 1.06870685E-11-1.16239667E+04 2.14697651E+01
 4
 C5H9O3r_15 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 7.69029944E+00 3.58564748E-02 2.07580896E-05-5.58540259E-08 2.61671705E-
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 C5H10O4_14 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
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 05 3
 1.87886725E-08-3.37013257E-12-6.27575930E+04 9.48161099E+00
 4
 C4H6O3_2 C 4 O 3 H 6 G 3E+02 1E+03 6E+02
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 05 3

-6.18204813E-08 2.64382111E-11-6.21910909E+04 5.97064458E+00
4
C5H11O5r_13 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
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11 2
-5.18199484E+04-3.13185304E+01 1.44716331E+01 2.68462509E-02 4.36279795E-
05 3
-7.16673308E-08 2.90444557E-11-5.18199484E+04-3.13185304E+01
4
C5H10O3_6 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
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04 3
-2.38372550E-07 1.02089263E-10-6.17025117E+04-2.16638527E+01
4
C5H9O3r_10 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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05 3
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C5H10O3 C 5 O 3 H 10 G 3E+02 1E+03 6E+02
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-4.17182269E+04 1.34294190E+01 4.05810474E+00 6.59957498E-02-5.55999993E-
05 3
3.34227393E-08-1.07364104E-11-4.17182269E+04 1.34294190E+01
4
C5H11O5r_37 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
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05 3
-8.37829051E-08 3.33793926E-11-5.06298949E+04-2.92056655E+01
4
C5H7O3r_Olef_4 C 5 O 3 H 7 G 3E+02 1E+03 6E+02
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-4.26771703E+04 2.82294867E+01-8.48568693E-01 1.08685436E-01-1.78583308E-
04 3
1.62986196E-07-5.78658300E-11-4.26771703E+04 2.82294867E+01
4
C5H8O2_Olef_3 C 5 O 2 H 8 G 3E+02 1E+03 6E+02
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6.95509637E+00 2.11365140E-02 4.63541985E-05-7.50358749E-08 3.12278838E-
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05 3
-7.50358749E-08 3.12278838E-11-3.89025916E+04 8.76296842E-01
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 -2.92579463E+04 2.74974071E+01-6.68435200E-01 1.04969353E-01-1.30059733E-
 04 3
 9.22922437E-08-2.76202448E-11-2.92579463E+04 2.74974071E+01
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 C4H7Or_Olef C 4 O 1 H 7 G 3E+02 1E+03 6E+02
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 3.94962071E+00 3.05829343E-02-3.16641839E-06-1.57036898E-08 8.28885786E-
 12 2
 7.10029065E+03 1.21333932E+01 3.94962071E+00 3.05829343E-02-3.16641839E-
 06 3
 -1.57036898E-08 8.28885786E-12 7.10029065E+03 1.21333932E+01
 4
 C5H9O3r_7 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
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 05 3
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 C4H7O2r_6 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
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 13 2
 -2.41759335E+04 2.48677143E+01 1.13808670E+00 4.45552970E-02-2.47315054E-
 05 3
 5.57451560E-09-1.33318072E-13-2.41759335E+04 2.48677143E+01
 4
 C5H9O5r_Olef_13 C 5 O 5 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -2.75964656E+04-5.42228937E+01 1.97686064E+01-7.43758860E-03 1.02348504E-
 04 3
 -1.14543138E-07 3.98811777E-11-2.75964656E+04-5.42228937E+01
 4
 C5H11O3r_21 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
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 04 3
 6.82201386E-08-2.05004328E-11-2.69002880E+04 2.21820682E+01
 4
 C5H10O4_8 C 5 O 4 H 10 G 3E+02 1E+03 6E+02
 1
 1.49301970E+00 8.94099829E-02-9.43395460E-05 6.28549184E-08-1.92615803E-
 11 2
 -7.60791075E+04 2.34708884E+01 1.49301970E+00 8.94099829E-02-9.43395460E-
 05 3
 6.28549184E-08-1.92615803E-11-7.60791075E+04 2.34708884E+01
 4
 C*CCCOH C 4 O 1 H 8 G 3E+02 1E+03 6E+02
 1

3.01991296E+00 3.40455054E-02-1.61611631E-06-1.99138933E-08 1.01683877E-
 11 2
 -2.11564864E+04 1.54017463E+01 3.01991296E+00 3.40455054E-02-1.61611631E-
 06 3
 -1.99138933E-08 1.01683877E-11-2.11564864E+04 1.54017463E+01
 4
 C4H7O2r_4 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 3.99595735E+00 3.27484593E-02 1.37559453E-05-4.47827621E-08 2.13214344E-
 11 2
 -2.92203209E+04 1.07819680E+01 3.99595735E+00 3.27484593E-02 1.37559453E-
 05 3
 -4.47827621E-08 2.13214344E-11-2.92203209E+04 1.07819680E+01
 4
 C5H11O5r_2 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 2.65922726E+00 1.12886119E-01-1.67293445E-04 1.48639455E-07-5.36413753E-
 11 2
 -4.28995007E+04 2.27010924E+01 2.65922726E+00 1.12886119E-01-1.67293445E-
 04 3
 1.48639455E-07-5.36413753E-11-4.28995007E+04 2.27010924E+01
 4
 C5H11O5r_25 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 1.62684721E+01 1.54338787E-02 6.55472778E-05-8.86608949E-08 3.38027950E-
 11 2
 -4.93634200E+04-3.60044935E+01 1.62684721E+01 1.54338787E-02 6.55472778E-
 05 3
 -8.86608949E-08 3.38027950E-11-4.93634200E+04-3.60044935E+01
 4
 C4H8O2_Olef_1 C 4 O 2 H 8 G 3E+02 1E+03 6E+02
 1
 6.73293549E-01 6.46071309E-02-5.88450535E-05 2.57942495E-08-3.50208075E-
 12 2
 -4.50314953E+04 2.33612156E+01 6.73293549E-01 6.46071309E-02-5.88450535E-
 05 3
 2.57942495E-08-3.50208075E-12-4.50314953E+04 2.33612156E+01
 4
 C5H12O C 5 O 1 H 12 G 3E+02 1E+03 6E+02
 1
 3.27098132E+00 4.99851562E-02-6.58276767E-06-2.37881850E-08 1.28054465E-
 11 2
 -4.07125177E+04 1.39383131E+01 3.27098132E+00 4.99851562E-02-6.58276767E-
 06 3
 -2.37881850E-08 1.28054465E-11-4.07125177E+04 1.39383131E+01
 4
 C4H7O2r C 4 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 1.94101363E+00 4.85187673E-02-2.82805945E-05 6.24514813E-10 4.21872854E-
 12 2
 -2.14184191E+04 1.88126357E+01 1.94101363E+00 4.85187673E-02-2.82805945E-
 05 3
 6.24514813E-10 4.21872854E-12-2.14184191E+04 1.88126357E+01
 4
 C5H11O5r_16 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
 1
 1.62684721E+01 1.54338787E-02 6.55472778E-05-8.86608949E-08 3.38027950E-
 11 2

-4.93634200E+04-3.60044935E+01 1.62684721E+01 1.54338787E-02 6.55472778E-05 3
-8.86608949E-08 3.38027950E-11-4.93634200E+04-3.60044935E+01
4
C5H7O3r_Olef_1 C 5 O 3 H 7 G 3E+02 1E+03 6E+02
1
6.61335959E+00 2.93663102E-02 3.50956871E-05-6.77034167E-08 2.85562117E-11 2
-3.49725321E+04 1.89566196E+00 6.61335959E+00 2.93663102E-02 3.50956871E-05 3
-6.77034167E-08 2.85562117E-11-3.49725321E+04 1.89566196E+00
4
CC(C)CC*O C 5 O 1 H 10 G 3E+02 1E+03 6E+02
1
4.34606546E+00 3.38467979E-02 1.93851708E-05-4.45356868E-08 1.90675600E-11 2
-3.14720619E+04 9.58596697E+00 4.34606546E+00 3.38467979E-02 1.93851708E-05 3
-4.45356868E-08 1.90675600E-11-3.14720619E+04 9.58596697E+00
4
CC(C)*CC*O C 5 O 1 H 8 G 3E+02 1E+03 6E+02
1
-2.84243863E+00 9.22410292E-02-1.34745291E-04 1.13693573E-07-3.84218263E-11 2
-2.00565909E+04 3.49995525E+01-2.84243863E+00 9.22410292E-02-1.34745291E-04 3
1.13693573E-07-3.84218263E-11-2.00565909E+04 3.49995525E+01
4
C5H11O3r_8 C 5 O 3 H 11 G 3E+02 1E+03 6E+02
1
3.42013911E+00 8.25801260E-02-9.02524375E-05 6.33421488E-08-2.00770305E-11 2
-2.56338131E+04 1.60763874E+01 3.42013911E+00 8.25801260E-02-9.02524375E-05 3
6.33421488E-08-2.00770305E-11-2.56338131E+04 1.60763874E+01
4
C5H9O2r_3 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
1
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-2.43101477E+04 3.06474732E+01-1.31901606E-02 6.45803907E-02-4.87586136E-05 3
2.17753053E-08-4.64243853E-12-2.43101477E+04 3.06474732E+01
4
C5H11O5r_39 C 5 O 5 H 11 G 3E+02 1E+03 6E+02
1
1.42954998E+01 2.34210633E-02 5.50592769E-05-8.37829051E-08 3.33793926E-11 2
-5.06298949E+04-2.92056655E+01 1.42954998E+01 2.34210633E-02 5.50592769E-05 3
-8.37829051E-08 3.33793926E-11-5.06298949E+04-2.92056655E+01
4
C6H13Or_1 C 6 O 1 H 13 G 3E+02 1E+03 6E+02
1
2.56257729E+00 5.74034811E-02-5.65327902E-06-3.11708729E-08 1.65745366E-11 2
-2.15334586E+04 1.87834933E+01 2.56257729E+00 5.74034811E-02-5.65327902E-06 3

-3.11708729E-08 1.65745366E-11-2.15334586E+04 1.87834933E+01
 4
 C5H9O5r_Olef_7 C 5 O 5 H 9 G 3E+02 1E+03 6E+02
 1
 -7.78377805E+00 1.83705788E-01-3.32700218E-04 3.02293367E-07-1.05312000E-
 10 2
 -3.25254114E+04 5.95077272E+01-7.78377805E+00 1.83705788E-01-3.32700218E-
 04 3
 3.02293367E-07-1.05312000E-10-3.25254114E+04 5.95077272E+01
 4
 C4H7O2r_Olef C 4 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 -2.07735433E+00 8.40259726E-02-1.14350974E-04 8.83098381E-08-2.84450728E-
 11 2
 1.32282768E+03 3.34773089E+01-2.07735433E+00 8.40259726E-02-1.14350974E-
 04 3
 8.83098381E-08-2.84450728E-11 1.32282768E+03 3.34773089E+01
 4
 C5H8O_Olef_4 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 -2.14728762E-02 6.95686527E-02-8.36688988E-05 6.52141762E-08-2.17278234E-
 11 2
 -2.17075359E+04 2.63770073E+01-2.14728762E-02 6.95686527E-02-8.36688988E-
 05 3
 6.52141762E-08-2.17278234E-11-2.17075359E+04 2.63770073E+01
 4
 C5H9O3r_Olef_73 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -1.18475103E+00 1.04775997E-01-1.56811256E-04 1.33893381E-07-4.59033222E-
 11 2
 -1.81448268E+04 3.54038746E+01-1.18475103E+00 1.04775997E-01-1.56811256E-
 04 3
 1.33893381E-07-4.59033222E-11-1.81448268E+04 3.54038746E+01
 4
 C5H9Or_Olef_14 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 2.80114172E+00 4.75042552E-02-1.48268828E-05-1.63628425E-08 1.10590175E-
 11 2
 -1.29207536E+02 1.66433097E+01 2.80114172E+00 4.75042552E-02-1.48268828E-
 05 3
 -1.63628425E-08 1.10590175E-11-1.29207536E+02 1.66433097E+01
 4
 C*CCCCJ C 5 H 9 G 3E+02 1E+03 6E+02
 1
 -3.65077001E-01 5.38600000E-02-3.68800000E-05 1.29800000E-08-1.78400000E-
 12 2
 2.08000000E+04 3.12000000E+01-3.65077001E-01 5.38600000E-02-3.68800000E-
 05 3
 1.29800000E-08-1.78400000E-12 2.08000000E+04 3.12000000E+01
 4
 C6H11r_Olef_13 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 5.39161188E+00 2.72345205E-02 4.07670604E-05-6.68588638E-08 2.71765750E-
 11 2
 1.56949628E+04 7.54968727E+00 5.39161188E+00 2.72345205E-02 4.07670604E-
 05 3
 -6.68588638E-08 2.71765750E-11 1.56949628E+04 7.54968727E+00
 4

C5H9O3r_Olef_112 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.71567902E+00 9.53828366E-02-1.49190818E-04 1.34018142E-07-4.74530530E-
 11 2
 -1.74921113E+04 1.99344121E+01 1.71567902E+00 9.53828366E-02-1.49190818E-
 04 3
 1.34018142E-07-4.74530530E-11-1.74921113E+04 1.99344121E+01
 4
 C6H11r_Olef_9 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 3.09131819E+00 4.43547750E-02 7.76904902E-06-4.06241976E-08 1.95180979E-
 11 2
 1.52137275E+04 1.14700560E+01 3.09131819E+00 4.43547750E-02 7.76904902E-
 06 3
 -4.06241976E-08 1.95180979E-11 1.52137275E+04 1.14700560E+01
 4
 C5H9O3r_Olef_106 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -4.50334946E+00 1.32225852E-01-2.23139579E-04 1.99005712E-07-6.87646195E-
 11 2
 -1.86902603E+04 4.58002991E+01-4.50334946E+00 1.32225852E-01-2.23139579E-
 04 3
 1.99005712E-07-6.87646195E-11-1.86902603E+04 4.58002991E+01
 4
 C5H9Or_Olef_19 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 2.12619517E+00 4.89917474E-02-1.78233486E-05-1.13177934E-08 8.48406933E-
 12 2
 -7.06567204E+03 1.98204931E+01 2.12619517E+00 4.89917474E-02-1.78233486E-
 05 3
 -1.13177934E-08 8.48406933E-12-7.06567204E+03 1.98204931E+01
 4
 C5H9Or_Olef_42 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -2.62321976E+00 8.47522652E-02-9.62292340E-05 6.05435537E-08-1.55977357E-
 11 2
 -1.18332730E+04 3.33354057E+01-2.62321976E+00 8.47522652E-02-9.62292340E-
 05 3
 6.05435537E-08-1.55977357E-11-1.18332730E+04 3.33354057E+01
 4
 C4H7O2r_Olef_2 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 2.15987066E-01 7.10312060E-02-9.25677754E-05 7.21062608E-08-2.39305494E-
 11 2
 1.02205416E+04 2.77990005E+01 2.15987066E-01 7.10312060E-02-9.25677754E-
 05 3
 7.21062608E-08-2.39305494E-11 1.02205416E+04 2.77990005E+01
 4
 C6H11r_Olef_4 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 -6.71564001E-01 7.16300000E-02-5.70000000E-05 2.48000000E-08-4.49300000E-
 12 2
 1.58700000E+04 2.98200000E+01-6.71564001E-01 7.16300000E-02-5.70000000E-
 05 3
 2.48000000E-08-4.49300000E-12 1.58700000E+04 2.98200000E+01
 4
 C5H9Or_Olef_37 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1

-1.19488451E+00 8.30360224E-02-1.03653686E-04 7.42993861E-08-2.19407006E-
 11 2
 -2.99413688E+03 2.87875268E+01-1.19488451E+00 8.30360224E-02-1.03653686E-
 04 3
 7.42993861E-08-2.19407006E-11-2.99413688E+03 2.87875268E+01
 4
 C5H9O3r_Olef_115 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -2.38090801E+00 1.21831370E-01-1.97101798E-04 1.70559979E-07-5.77706680E-
 11 2
 -1.82148670E+04 3.56771589E+01-2.38090801E+00 1.21831370E-01-1.97101798E-
 04 3
 1.70559979E-07-5.77706680E-11-1.82148670E+04 3.56771589E+01
 4
 C5H9O3r_Olef_47 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -3.63363935E-01 1.05132500E-01-1.58275464E-04 1.33433625E-07-4.49516237E-
 11 2
 -1.78928957E+04 2.84544066E+01-3.63363935E-01 1.05132500E-01-1.58275464E-
 04 3
 1.33433625E-07-4.49516237E-11-1.78928957E+04 2.84544066E+01
 4
 C5H9Or_Olef_17 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -3.00502813E-01 6.36102151E-02-3.80336672E-05-2.25257362E-09 7.86203866E-
 12 2
 -2.80997865E+03 2.97443718E+01-3.00502813E-01 6.36102151E-02-3.80336672E-
 05 3
 -2.25257362E-09 7.86203866E-12-2.80997865E+03 2.97443718E+01
 4
 C5H9O3r_Olef_93 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -1.97910112E+00 1.13614233E-01-1.74883686E-04 1.47419493E-07-4.93251599E-
 11 2
 -2.03617100E+04 3.50015992E+01-1.97910112E+00 1.13614233E-01-1.74883686E-
 04 3
 1.47419493E-07-4.93251599E-11-2.03617100E+04 3.50015992E+01
 4
 C5H9Or_Olef_13 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 3.93790277E-01 6.61597153E-02-5.60723529E-05 2.21959060E-08-2.14288409E-
 12 2
 -1.58193283E+03 2.55101692E+01 3.93790277E-01 6.61597153E-02-5.60723529E-
 05 3
 2.21959060E-08-2.14288409E-12-1.58193283E+03 2.55101692E+01
 4
 C5H9O3r_Olef_90 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 2.03568611E+00 8.25506440E-02-9.48924176E-05 6.73058407E-08-2.12042425E-
 11 2
 -1.00359438E+04 1.86994540E+01 2.03568611E+00 8.25506440E-02-9.48924176E-
 05 3
 6.73058407E-08-2.12042425E-11-1.00359438E+04 1.86994540E+01
 4
 C5H9Or_Olef_24 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 6.19797769E+00 2.63045835E-02 1.56702821E-05-2.86305310E-08 1.05190933E-
 11 2

2.36377652E+03 2.13761515E+00 6.19797769E+00 2.63045835E-02 1.56702821E-05 3
-2.86305310E-08 1.05190933E-11 2.36377652E+03 2.13761515E+00
4
C5H9O3r_Olef_71 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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-4.57902579E+00 1.32324118E-01-2.13604837E-04 1.82363096E-07-6.10922407E-11 2
-1.95869698E+04 4.48447982E+01-4.57902579E+00 1.32324118E-01-2.13604837E-04 3
1.82363096E-07-6.10922407E-11-1.95869698E+04 4.48447982E+01
4
C5H9O3r_Olef_124 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-9.97766764E-01 1.03819073E-01-1.48823434E-04 1.21386915E-07-4.03128959E-11 2
-2.22430563E+04 2.95349274E+01-9.97766764E-01 1.03819073E-01-1.48823434E-04 3
1.21386915E-07-4.03128959E-11-2.22430563E+04 2.95349274E+01
4
C5H6O_Olef_3 C 5 O 1 H 6 G 3E+02 1E+03 6E+02
1
-5.24212547E-01 5.86250077E-02-5.81718213E-05 3.33006972E-08-8.10331938E-12 2
-2.92651138E+03 2.83975412E+01-5.24212547E-01 5.86250077E-02-5.81718213E-05 3
3.33006972E-08-8.10331938E-12-2.92651138E+03 2.83975412E+01
4
C5H9O3r_Olef_24 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-1.93678354E+00 1.00435239E-01-1.16768435E-04 7.41079959E-08-1.99888838E-11 2
-2.40941142E+04 3.32349174E+01-1.93678354E+00 1.00435239E-01-1.16768435E-04 3
7.41079959E-08-1.99888838E-11-2.40941142E+04 3.32349174E+01
4
C5H9r_Olef_3 C 5 H 9 G 3E+02 1E+03 6E+02
1
5.37065769E+00 1.72018365E-02 4.58055906E-05-6.83486669E-08 2.75991543E-11 2
1.83892148E+04 5.31577492E+00 5.37065769E+00 1.72018365E-02 4.58055906E-05 3
-6.83486669E-08 2.75991543E-11 1.83892148E+04 5.31577492E+00
4
C5H9O3r_Olef_60 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
1.03078645E+00 9.20753817E-02-1.26478738E-04 1.02441565E-07-3.41666220E-11 2
-1.88779888E+04 2.36111627E+01 1.03078645E+00 9.20753817E-02-1.26478738E-04 3
1.02441565E-07-3.41666220E-11-1.88779888E+04 2.36111627E+01
4
C5H9O3r_Olef_99 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-2.80701028E+00 1.10058996E-01-1.45570580E-04 1.03713953E-07-3.06336403E-11 2
-2.30751091E+04 3.88376403E+01-2.80701028E+00 1.10058996E-01-1.45570580E-04 3

1.03713953E-07-3.06336403E-11-2.30751091E+04 3.88376403E+01
 4
 C5H6O_Olef_1 C 5 O 1 H 6 G 3E+02 1E+03 6E+02
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 -4.22577303E+03 4.78411122E+01-5.60395793E+00 9.66315214E-02-1.31318303E-04 3
 9.62748696E-08-2.87375144E-11-4.22577303E+03 4.78411122E+01
 4
 C*C(CP)C*C C 5 O 2 H 8 G 3E+02 1E+03 6E+02
 1
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 -1.94829735E+03 3.21702795E+01-1.24103433E+00 9.45520538E-02-1.42511939E-04 3
 1.22302353E-07-4.21545834E-11-1.94829735E+03 3.21702795E+01
 4
 C5H9O3r_Olef_108 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -4.90347292E+00 1.22016526E-01-1.68484704E-04 1.22778134E-07-3.65473385E-11 2
 -2.13706286E+04 4.99827075E+01-4.90347292E+00 1.22016526E-01-1.68484704E-04 3
 1.22778134E-07-3.65473385E-11-2.13706286E+04 4.99827075E+01
 4
 C5H9O3r_Olef_125 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 -2.41275619E+04 4.94453584E+01-6.08669728E+00 1.35107587E-01-2.06313028E-04 3
 1.65780325E-07-5.29700046E-11-2.41275619E+04 4.94453584E+01
 4
 C6H11r_Olef_5 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 5.03959177E+00 2.82930864E-02 4.20819586E-05-6.99156864E-08 2.86065052E-11 2
 7.14666488E+03 4.78791125E+00 5.03959177E+00 2.82930864E-02 4.20819586E-05 3
 -6.99156864E-08 2.86065052E-11 7.14666488E+03 4.78791125E+00
 4
 C5H10_Olef_1 C 5 H 10 G 3E+02 1E+03 6E+02
 1
 8.35361995E-02 4.71500000E-02-1.66100000E-05-4.16300002E-09 2.98000000E-12 2
 -4.93800000E+03 2.75800000E+01 8.35361995E-02 4.71500000E-02-1.66100000E-05 3
 -4.16300002E-09 2.98000000E-12-4.93800000E+03 2.75800000E+01
 4
 C6H11r_Olef_3 C 6 H 11 G 3E+02 1E+03 6E+02
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 7.55300000E+03 3.13200000E+01-5.99756001E-01 6.26300000E-02-3.69500000E-05 3
 9.44099997E-09-4.81199998E-13 7.55300000E+03 3.13200000E+01
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C5H9Or_Olef_23 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 12 2
 -2.05304900E+03 1.59959822E+01 3.19845786E+00 4.88868135E-02-2.11378696E-
 05 3
 -8.01012114E-09 7.47311203E-12-2.05304900E+03 1.59959822E+01
 4
 C5H9O3r_Olef_119 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -1.82148670E+04 3.56771589E+01-2.38090801E+00 1.21831370E-01-1.97101798E-
 04 3
 1.70559979E-07-5.77706680E-11-1.82148670E+04 3.56771589E+01
 4
 C5H8O_Olef_7 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -1.91991068E+04 8.28274032E+00 4.40877340E+00 2.49440409E-02 2.98452010E-
 05 3
 -5.19638650E-08 2.12276798E-11-1.91991068E+04 8.28274032E+00
 4
 C5H9O3r_Olef_35 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -2.14352853E+04 3.97244937E+01-3.16990574E+00 1.15874869E-01-1.62202817E-
 04 3
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 4
 C6H11r_Olef_15 C 6 H 11 G 3E+02 1E+03 6E+02
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 12 2
 1.62255803E+04 3.03483787E+01-1.48961271E-01 6.48365229E-02-4.03151599E-
 05 3
 7.87008511E-09 1.82758315E-12 1.62255803E+04 3.03483787E+01
 4
 C5H9O3r_Olef_67 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -2.10486574E+04 4.27599552E+01-2.88592885E+00 1.05317656E-01-1.29658369E-
 04 3
 8.56517800E-08-2.37282942E-11-2.10486574E+04 4.27599552E+01
 4
 C*CCC*C C 5 H 8 G 3E+02 1E+03 6E+02
 1
 1.81322000E+00 3.99800000E-02-1.65700000E-05-1.06000002E-09 1.81800000E-
 12 2
 1.07400000E+04 1.83600000E+01 1.81322000E+00 3.99800000E-02-1.65700000E-
 05 3
 -1.06000002E-09 1.81800000E-12 1.07400000E+04 1.83600000E+01
 4
 C5H9Or_Olef_22 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 11 2
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 4
 C5H9O3r_Olef_56 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 1.03078645E+00 9.20753817E-02-1.26478738E-04 1.02441565E-07-3.41666220E-
 11 2
 -1.88779888E+04 2.36111627E+01 1.03078645E+00 9.20753817E-02-1.26478738E-
 04 3
 1.02441565E-07-3.41666220E-11-1.88779888E+04 2.36111627E+01
 4
 C5H6O_Olef C 5 O 1 H 6 G 3E+02 1E+03 6E+02
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 11 2
 -6.82821027E+03 4.97485714E+01-6.23115146E+00 1.23032844E-01-2.25380031E-
 04 3
 2.09709125E-07-7.39281221E-11-6.82821027E+03 4.97485714E+01
 4
 C5H9Or_Olef_38 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
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 12 2
 -9.15073687E+01 1.40667069E+01 2.92768133E+00 5.81505375E-02-5.26190494E-
 05 3
 2.83759972E-08-6.54283236E-12-9.15073687E+01 1.40667069E+01
 4
 C5H9Or_Olef_16 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 12 2
 -9.80682131E+03 3.72577206E+01-2.70213834E+00 8.00109257E-02-8.03170236E-
 05 3
 4.24813808E-08-8.69238965E-12-9.80682131E+03 3.72577206E+01
 4
 C5H9Or_Olef_10 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -1.97862129E-01 7.49737719E-02-7.29172561E-05 3.72957548E-08-7.32229461E-
 12 2
 -1.27293694E+04 2.22636673E+01-1.97862129E-01 7.49737719E-02-7.29172561E-
 05 3
 3.72957548E-08-7.32229461E-12-1.27293694E+04 2.22636673E+01
 4
 C5H9O3r_Olef_111 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -3.10919908E+00 1.19168733E-01-1.91342854E-04 1.68013653E-07-5.79796178E-
 11 2
 -1.96753534E+04 4.09570552E+01-3.10919908E+00 1.19168733E-01-1.91342854E-
 04 3
 1.68013653E-07-5.79796178E-11-1.96753534E+04 4.09570552E+01
 4
 C5H9O3r_Olef_78 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 9.37690427E-01 9.43815147E-02-1.30773475E-04 1.05447648E-07-3.49093707E-
 11 2

-1.76694334E+04 2.52807345E+01 9.37690427E-01 9.43815147E-02-1.30773475E-
04 3
1.05447648E-07-3.49093707E-11-1.76694334E+04 2.52807345E+01
4
C5H9O3r_Olef_84 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
3.90989259E+00 7.29445385E-02-8.43117439E-05 6.68055506E-08-2.36887938E-
11 2
-1.03096246E+04 1.16773591E+01 3.90989259E+00 7.29445385E-02-8.43117439E-
05 3
6.68055506E-08-2.36887938E-11-1.03096246E+04 1.16773591E+01
4
C5H9Or_Olef_15 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
2.33454633E+00 4.22451549E-02 6.05835759E-06-3.84168193E-08 1.86077852E-
11 2
-1.60796833E+04 1.65537446E+01 2.33454633E+00 4.22451549E-02 6.05835759E-
06 3
-3.84168193E-08 1.86077852E-11-1.60796833E+04 1.65537446E+01
4
C5H9O3r_Olef_32 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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11 2
-2.02166046E+04 3.34572423E+01-1.07668534E+00 9.90777330E-02-1.32911224E-
04 3
1.03324742E-07-3.34075499E-11-2.02166046E+04 3.34572423E+01
4
C5H9O3r_Olef_29 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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-3.07680972E+00 1.13568736E-01-1.57908080E-04 1.20802398E-07-3.78114667E-
11 2
-2.26438407E+04 3.80549220E+01-3.07680972E+00 1.13568736E-01-1.57908080E-
04 3
1.20802398E-07-3.78114667E-11-2.26438407E+04 3.80549220E+01
4
C5H9O3r_Olef_40 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-1.61239120E+00 1.05297543E-01-1.38312412E-04 1.02912585E-07-3.20663895E-
11 2
-9.45807710E+03 3.34940087E+01-1.61239120E+00 1.05297543E-01-1.38312412E-
04 3
1.02912585E-07-3.20663895E-11-9.45807710E+03 3.34940087E+01
4
C5H10O2_Olef_12 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
-2.00958949E+00 1.02202509E-01-1.37647741E-04 1.07637699E-07-3.49924650E-
11 2
-1.81155373E+04 3.32363433E+01-2.00958949E+00 1.02202509E-01-1.37647741E-
04 3
1.07637699E-07-3.49924650E-11-1.81155373E+04 3.32363433E+01
4
C5H9O3r_Olef_51 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
3.90989259E+00 7.29445385E-02-8.43117439E-05 6.68055506E-08-2.36887938E-
11 2
-1.03096246E+04 1.16773591E+01 3.90989259E+00 7.29445385E-02-8.43117439E-
05 3

6.68055506E-08-2.36887938E-11-1.03096246E+04 1.16773591E+01
4
C3H5Or_Olef C 3 O 1 H 5 G 3E+02 1E+03 6E+02
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-1.93204234E+00 5.67834808E-02-7.00581349E-05 4.57824258E-08-1.19624898E-
11 2
-2.20603581E+03 3.16848944E+01-1.93204234E+00 5.67834808E-02-7.00581349E-
05 3
4.57824258E-08-1.19624898E-11-2.20603581E+03 3.16848944E+01
4
C5H10O2_Olef_8 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
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-3.00193298E+00 1.07042491E-01-1.47226355E-04 1.15489273E-07-3.73319587E-
11 2
-1.78178687E+04 3.74040274E+01-3.00193298E+00 1.07042491E-01-1.47226355E-
04 3
1.15489273E-07-3.73319587E-11-1.78178687E+04 3.74040274E+01
4
C5H9Or_Olef_29 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
4.19785331E+00 4.07955866E-02-9.32657379E-06-1.11528754E-08 6.11517657E-
12 2
-6.34596178E+01 6.73529480E+00 4.19785331E+00 4.07955866E-02-9.32657379E-
06 3
-1.11528754E-08 6.11517657E-12-6.34596178E+01 6.73529480E+00
4
C5H9O3r_Olef_89 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-1.97910112E+00 1.13614233E-01-1.74883686E-04 1.47419493E-07-4.93251599E-
11 2
-1.89022914E+04 3.50015992E+01-1.97910112E+00 1.13614233E-01-1.74883686E-
04 3
1.47419493E-07-4.93251599E-11-1.89022914E+04 3.50015992E+01
4
C5H7Or_Olef_1 C 5 O 1 H 7 G 3E+02 1E+03 6E+02
1
3.51537696E+00 3.54364152E-02 3.18505947E-06-2.79870617E-08 1.32980592E-
11 2
1.61681427E+04 1.32540845E+01 3.51537696E+00 3.54364152E-02 3.18505947E-
06 3
-2.79870617E-08 1.32980592E-11 1.61681427E+04 1.32540845E+01
4
C5H9O3r_Olef_36 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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2.24369023E-01 8.83267476E-02-1.05409235E-04 7.53387654E-08-2.33652969E-
11 2
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04 3
7.53387654E-08-2.33652969E-11-1.99931423E+04 3.02835701E+01
4
C5H9O3r_Olef_129 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-9.86757624E-01 1.08774251E-01-1.65305073E-04 1.39567919E-07-4.69856663E-
11 2
-1.91999601E+04 3.08339150E+01-9.86757624E-01 1.08774251E-01-1.65305073E-
04 3
1.39567919E-07-4.69856663E-11-1.91999601E+04 3.08339150E+01
4

C5H9Or_Olef_32 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -1.39789782E+02 1.60692457E+01 3.78806504E+00 3.86115937E-02 7.21228467E-
 07 3
 -2.62738091E-08 1.30460344E-11-1.39789782E+02 1.60692457E+01
 4
 C6H11r_Olef C 6 H 11 G 3E+02 1E+03 6E+02
 1
 3.11514372E+00 4.26858230E-02 7.55036095E-06-3.57954152E-08 1.65302096E-
 11 2
 5.61613822E+03 1.07465569E+01 3.11514372E+00 4.26858230E-02 7.55036095E-
 06 3
 -3.57954152E-08 1.65302096E-11 5.61613822E+03 1.07465569E+01
 4
 C*CCJCC C 5 H 9 G 3E+02 1E+03 6E+02
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 13 2
 1.19500000E+04 2.84100000E+01-2.78104001E-01 5.27800000E-02-3.34800000E-
 05 3
 1.00400000E-08-9.55400002E-13 1.19500000E+04 2.84100000E+01
 4
 C5H9Or_Olef_9 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 1.47293527E+00 6.47590591E-02-5.68377264E-05 2.42227999E-08-2.96374991E-
 12 2
 -1.51343112E+03 1.76158335E+01 1.47293527E+00 6.47590591E-02-5.68377264E-
 05 3
 2.42227999E-08-2.96374991E-12-1.51343112E+03 1.76158335E+01
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 C5H9O3r_Olef_123 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -2.22430563E+04 2.95349274E+01-9.97766764E-01 1.03819073E-01-1.48823434E-
 04 3
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 11 2
 -2.44160854E+04 4.04576697E+01-3.95432761E+00 1.17134108E-01-1.55594770E-
 04 3
 1.11234350E-07-3.28079282E-11-2.44160854E+04 4.04576697E+01
 4
 C5H9O3r_Olef_128 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -1.06315958E+04 1.89001114E+01 1.89234852E+00 8.96434081E-02-1.23138078E-
 04 3
 1.03931905E-07-3.65078382E-11-1.06315958E+04 1.89001114E+01
 4
 C*CCCC C 5 H 10 G 3E+02 1E+03 6E+02
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 11 2
 -4.89670267E+03 1.22015626E+01 3.59709404E+00 2.81126994E-02 2.86626078E-
 05 3
 -5.29107130E-08 2.20767194E-11-4.89670267E+03 1.22015626E+01
 4
 C5H9O3r_Olef_38 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -8.01593406E+03 2.40530852E+01 1.78188356E+00 7.77494214E-02-8.15188310E-
 05 3
 5.44428702E-08-1.68774710E-11-8.01593406E+03 2.40530852E+01
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 C5H9O3r_Olef_87 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 12 2
 -8.92540100E+03 1.07048352E+01 5.23809904E+00 5.56897346E-02-4.23009004E-
 05 3
 2.62199083E-08-9.66602645E-12-8.92540100E+03 1.07048352E+01
 4
 C5H10O2_Olef_9 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
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 11 2
 -1.73927816E+04 1.74935964E+01 2.08699754E+00 7.57539763E-02-8.97367612E-
 05 3
 7.10958625E-08-2.46748500E-11-1.73927816E+04 1.74935964E+01
 4
 C5H9Or_Olef_41 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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 11 2
 -8.82978632E+03 3.50978745E+01-3.28562366E+00 9.32387385E-02-1.13443265E-
 04 3
 7.42782758E-08-1.95238935E-11-8.82978632E+03 3.50978745E+01
 4
 C5H9r_Olef_2 C 5 H 9 G 3E+02 1E+03 6E+02
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 12 2
 1.04300000E+04 2.00300000E+01 1.49390000E+00 4.01700000E-02-9.71399997E-
 06 3
 -7.85100002E-09 3.78000000E-12 1.04300000E+04 2.00300000E+01
 4
 C*CCCJC C 5 H 9 G 3E+02 1E+03 6E+02
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 3.73057397E+00 2.10162674E-02 4.04468431E-05-6.32446774E-08 2.55287762E-
 11 2
 1.85454733E+04 1.43740042E+01 3.73057397E+00 2.10162674E-02 4.04468431E-
 05 3
 -6.32446774E-08 2.55287762E-11 1.85454733E+04 1.43740042E+01
 4
 C5H9Or_Olef_33 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 8.10963365E-01 6.67902054E-02-6.55322845E-05 3.77364391E-08-9.20627843E-
 12 2

-8.10703061E+03 2.07414221E+01 8.10963365E-01 6.67902054E-02-6.55322845E-
 05 3
 3.77364391E-08-9.20627843E-12-8.10703061E+03 2.07414221E+01
 4
 C5H7Or_Olef_3 C 5 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 2.94886439E+00 4.98440006E-02-5.30171062E-05 4.06381322E-08-1.38659862E-
 11 2
 1.57818091E+04 1.50892079E+01 2.94886439E+00 4.98440006E-02-5.30171062E-
 05 3
 4.06381322E-08-1.38659862E-11 1.57818091E+04 1.50892079E+01
 4
 C5H9O3r_Olef_109 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.01336675E+00 9.42832482E-02-1.40308217E-04 1.22090264E-07-4.25817495E-
 11 2
 -1.67727239E+04 2.62362354E+01 1.01336675E+00 9.42832482E-02-1.40308217E-
 04 3
 1.22090264E-07-4.25817495E-11-1.67727239E+04 2.62362354E+01
 4
 C5H9O3r_Olef_37 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 2.35899290E+00 7.48205778E-02-8.44678948E-05 6.18559227E-08-2.01438546E-
 11 2
 -1.74937652E+04 2.26386389E+01 2.35899290E+00 7.48205778E-02-8.44678948E-
 05 3
 6.18559227E-08-2.01438546E-11-1.74937652E+04 2.26386389E+01
 4
 C6H11r_Olef_11 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 5.01899000E+00 4.31900000E-02-1.07500000E-05-7.01300002E-09 3.42800000E-
 12 2
 1.46000000E+04 7.01300001E+00 5.01899000E+00 4.31900000E-02-1.07500000E-
 05 3
 -7.01300002E-09 3.42800000E-12 1.46000000E+04 7.01300001E+00
 4
 C3H5O2r_Olef C 3 O 2 H 5 G 3E+02 1E+03 6E+02
 1
 1.41841460E+00 3.63226697E-02-7.27053194E-06-2.31454738E-08 1.38803046E-
 11 2
 4.31384740E+03 2.17678370E+01 1.41841460E+00 3.63226697E-02-7.27053194E-
 06 3
 -2.31454738E-08 1.38803046E-11 4.31384740E+03 2.17678370E+01
 4
 C5H9O3r_Olef_63 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 -3.63363935E-01 1.05132500E-01-1.58275464E-04 1.33433625E-07-4.49516237E-
 11 2
 -1.78928957E+04 2.84544066E+01-3.63363935E-01 1.05132500E-01-1.58275464E-
 04 3
 1.33433625E-07-4.49516237E-11-1.78928957E+04 2.84544066E+01
 4
 C5H9O3r_Olef_80 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 1.79412100E+01-3.06188473E-02 1.58860829E-04-1.80322417E-07 6.77237180E-
 11 2
 -2.26912097E+04-4.28657750E+01 1.79412100E+01-3.06188473E-02 1.58860829E-
 04 3

-1.80322417E-07 6.77237180E-11-2.26912097E+04-4.28657750E+01
4
C4H7O2r_Olef_1 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
1
-5.98102596E-02 6.73271030E-02-7.55246398E-05 5.11834839E-08-1.56260285E-
11 2
1.64479892E+03 2.62545566E+01-5.98102596E-02 6.73271030E-02-7.55246398E-
05 3
5.11834839E-08-1.56260285E-11 1.64479892E+03 2.62545566E+01
4
C4H7O2r_Olef_3 C 4 O 2 H 7 G 3E+02 1E+03 6E+02
1
-2.76990811E-02 7.27504476E-02-9.50305249E-05 7.48145282E-08-2.50826988E-
11 2
-2.73828405E+02 2.50234989E+01-2.76990811E-02 7.27504476E-02-9.50305249E-
05 3
7.48145282E-08-2.50826988E-11-2.73828405E+02 2.50234989E+01
4
C4H6O_Olef_6 C 4 O 1 H 6 G 3E+02 1E+03 6E+02
1
1.92522377E+00 3.85165862E-02-1.86053968E-05-4.49720832E-09 5.25143217E-
12 2
-3.76406201E+03 1.74109956E+01 1.92522377E+00 3.85165862E-02-1.86053968E-
05 3
-4.49720832E-09 5.25143217E-12-3.76406201E+03 1.74109956E+01
4
C5H8O_Olef_2 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
1
1.01660534E+00 6.70156392E-02-8.06423865E-05 6.31750013E-08-2.11268581E-
11 2
-2.07970633E+04 2.17200850E+01 1.01660534E+00 6.70156392E-02-8.06423865E-
05 3
6.31750013E-08-2.11268581E-11-2.07970633E+04 2.17200850E+01
4
C5H8O_Olef_5 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
1
2.31231075E+00 3.69015710E-02 6.93107681E-06-3.28996838E-08 1.53139815E-
11 2
-1.74946264E+04 1.83291952E+01 2.31231075E+00 3.69015710E-02 6.93107681E-
06 3
-3.28996838E-08 1.53139815E-11-1.74946264E+04 1.83291952E+01
4
C6H11r_Olef_2 C 6 H 11 G 3E+02 1E+03 6E+02
1
1.07377412E+00 6.10536446E-02-3.10572855E-05-3.49784343E-09 6.69905355E-
12 2
1.48917562E+04 1.86928083E+01 1.07377412E+00 6.10536446E-02-3.10572855E-
05 3
-3.49784343E-09 6.69905355E-12 1.48917562E+04 1.86928083E+01
4
C5H10O2_Olef_10 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
-9.46510758E-03 8.77115063E-02-1.12650885E-04 9.01600437E-08-3.05885483E-
11 2
-1.56883012E+04 2.75400513E+01-9.46510758E-03 8.77115063E-02-1.12650885E-
04 3
9.01600437E-08-3.05885483E-11-1.56883012E+04 2.75400513E+01
4

C5H9O3r_Olef_75 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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 3.03091083E+00 7.75843787E-02-1.01481882E-04 8.49639095E-08-2.97627052E-
 11 2
 -1.64507527E+04 1.90134831E+01 3.03091083E+00 7.75843787E-02-1.01481882E-
 04 3
 8.49639095E-08-2.97627052E-11-1.64507527E+04 1.90134831E+01
 4
 C5H9Or_Olef_35 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -5.40806512E+00 1.03633220E-01-1.39481045E-04 1.02724009E-07-3.05178450E-
 11 2
 -9.30517969E+03 4.66073091E+01-5.40806512E+00 1.03633220E-01-1.39481045E-
 04 3
 1.02724009E-07-3.05178450E-11-9.30517969E+03 4.66073091E+01
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 C5H10O2_Olef_14 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
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 2.08699754E+00 7.57539763E-02-8.97367612E-05 7.10958625E-08-2.46748500E-
 11 2
 -1.73927816E+04 1.74935964E+01 2.08699754E+00 7.57539763E-02-8.97367612E-
 05 3
 7.10958625E-08-2.46748500E-11-1.73927816E+04 1.74935964E+01
 4
 C5H9Or_Olef_44 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 4.18043361E+00 4.30034531E-02-2.31560525E-05 8.49582318E-09-2.29995098E-
 12 2
 2.04180528E+03 9.36036743E+00 4.18043361E+00 4.30034531E-02-2.31560525E-
 05 3
 8.49582318E-09-2.29995098E-12 2.04180528E+03 9.36036743E+00
 4
 C5H9Or_Olef_20 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -3.29636795E+00 8.20257255E-02-7.80434949E-05 3.60546721E-08-5.53393363E-
 12 2
 -1.18269408E+04 4.03174254E+01-3.29636795E+00 8.20257255E-02-7.80434949E-
 05 3
 3.60546721E-08-5.53393363E-12-1.18269408E+04 4.03174254E+01
 4
 C5H9O3r_Olef_86 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1
 2.35899290E+00 7.48205778E-02-8.44678948E-05 6.18559227E-08-2.01438546E-
 11 2
 -1.74937652E+04 2.26386389E+01 2.35899290E+00 7.48205778E-02-8.44678948E-
 05 3
 6.18559227E-08-2.01438546E-11-1.74937652E+04 2.26386389E+01
 4
 C3H5Or_Olef_1 C 3 O 1 H 5 G 3E+02 1E+03 6E+02
 1
 5.57072407E-01 3.83360101E-02-2.74303384E-05 4.95285905E-09 2.15921992E-
 12 2
 -2.74959547E+03 2.19041603E+01 5.57072407E-01 3.83360101E-02-2.74303384E-
 05 3
 4.95285905E-09 2.15921992E-12-2.74959547E+03 2.19041603E+01
 4
 C5H9O3r_Olef_45 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
 1

-1.03528187E+00 1.02368699E-01-1.41261476E-04 1.10325638E-07-3.53327731E-11 2
-1.89359083E+04 3.20795624E+01-1.03528187E+00 1.02368699E-01-1.41261476E-04 3
1.10325638E-07-3.53327731E-11-1.89359083E+04 3.20795624E+01 4
C6H11r_Olef_10 C 6 H 11 G 3E+02 1E+03 6E+02
1
3.65353950E+00 3.87699397E-02 2.18818722E-05-5.39235752E-08 2.39666393E-11 2
6.35329073E+03 8.71748197E+00 3.65353950E+00 3.87699397E-02 2.18818722E-05 3
-5.39235752E-08 2.39666393E-11 6.35329073E+03 8.71748197E+00 4
C5H8O_Olef_8 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
1
3.62703632E+00 3.12046127E-02 1.63893794E-05-4.03462250E-08 1.75970146E-11 2
-2.06296735E+04 1.36652275E+01 3.62703632E+00 3.12046127E-02 1.63893794E-05 3
-4.03462250E-08 1.75970146E-11-2.06296735E+04 1.36652275E+01 4
C5H9O3r_Olef_95 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
1.71567902E+00 9.53828366E-02-1.49190818E-04 1.34018142E-07-4.74530530E-11 2
-1.74921113E+04 1.99344121E+01 1.71567902E+00 9.53828366E-02-1.49190818E-04 3
1.34018142E-07-4.74530530E-11-1.74921113E+04 1.99344121E+01 4
C5H9Or_Olef_26 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
4.10475729E+00 4.31017196E-02-1.36213107E-05-8.14679247E-09 5.37242780E-12 2
1.14509580E+03 8.40486650E+00 4.10475729E+00 4.31017196E-02-1.36213107E-05 3
-8.14679247E-09 5.37242780E-12 1.14509580E+03 8.40486650E+00 4
C5H9O3r_Olef_103 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
-6.50347384E+00 1.46716855E-01-2.48136435E-04 2.16483368E-07-7.31685363E-11 2
-2.11174965E+04 5.03979788E+01-6.50347384E+00 1.46716855E-01-2.48136435E-04 3
2.16483368E-07-7.31685363E-11-2.11174965E+04 5.03979788E+01 4
C5H9O3r_Olef_17 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
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1.84382428E+00 8.32378561E-02-9.90944817E-05 7.46896233E-08-2.48549449E-11 2
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7.46896233E-08-2.48549449E-11-1.03675441E+04 2.01457588E+01 4
C5H9O3r_Olef_117 C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
9.00005023E-01 9.44833894E-02-1.32716692E-04 1.11783478E-07-3.88473318E-11 2

-1.03339272E+04 2.30677956E+01 9.00005023E-01 9.44833894E-02-1.32716692E-
04 3
1.11783478E-07-3.88473318E-11-1.03339272E+04 2.30677956E+01
4
C5H9Or_Olef_34 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
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11 2
-1.33574674E+04 4.58706059E+01-5.22081600E+00 9.64184620E-02-1.12575093E-
04 3
7.01749432E-08-1.76102292E-11-1.33574674E+04 4.58706059E+01
4
C5H8O2_Olef(m0) C 5 O 2 H 8 G 3E+02 1E+03 6E+02
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11 2
-1.56196379E+03 3.03351561E+01-6.74521760E-01 8.01444684E-02-8.63097734E-
05 3
5.36771589E-08-1.49905380E-11-1.56196379E+03 3.03351561E+01
4
C5H9Or_Olef_5m3 C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
3.19641263E+00 4.74256504E-02-1.61236747E-05-1.11739603E-08 7.86662388E-
12 2
-1.12872264E+04 1.17241315E+01 3.19641263E+00 4.74256504E-02-1.61236747E-
05 3
-1.11739603E-08 7.86662388E-12-1.12872264E+04 1.17241315E+01
4
C5H10O2_Olef_4m4 C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
7.95458525E-03 8.55036398E-02-9.88214067E-05 7.05113451E-08-2.21734207E-
11 2
-1.77935661E+04 2.60135910E+01 7.95458525E-03 8.55036398E-02-9.88214067E-
05 3
7.05113451E-08-2.21734207E-11-1.77935661E+04 2.60135910E+01
4
C5H9O3r_Olef_13m C 5 O 3 H 9 G 3E+02 1E+03 6E+02
1
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11 2
-1.89359083E+04 3.20795624E+01-1.03528187E+00 1.02368699E-01-1.41261476E-
04 3
1.10325638E-07-3.53327731E-11-1.89359083E+04 3.20795624E+01
4
C5H10O2_Olef_1m C 5 O 2 H 10 G 3E+02 1E+03 6E+02
1
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11 2
-1.65850107E+04 2.65845504E+01-8.51414357E-02 8.78097728E-02-1.03116144E-
04 3
7.35174281E-08-2.29161695E-11-1.65850107E+04 2.65845504E+01
4
C5H9Or_Olef_1m C 5 O 1 H 9 G 3E+02 1E+03 6E+02
1
-5.44608800E-01 8.14579287E-02-9.56640609E-05 6.13491540E-08-1.57827942E-
11 2
-1.83540236E+03 2.48385858E+01-5.44608800E-01 8.14579287E-02-9.56640609E-
05 3

6.13491540E-08-1.57827942E-11-1.83540236E+03 2.48385858E+01
 4
 C5H8O2_Olef_2m C 5 O 2 H 8 G 3E+02 1E+03 6E+02
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 4
 C5H10O2_Olef_3m C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 2.00807896E+00 7.10126367E-02-7.38245508E-05 5.30336896E-08-1.77695039E-
 11 2
 -1.53663300E+04 2.03172990E+01 2.00807896E+00 7.10126367E-02-7.38245508E-
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 5.30336896E-08-1.77695039E-11-1.53663300E+04 2.03172990E+01
 4
 C5H8O_Olef(m14) C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
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 11 2
 -1.80301392E+04 3.78232551E+01-2.92135721E+00 8.74996896E-02-1.18833081E-
 04 3
 9.56314003E-08-3.15164803E-11-1.80301392E+04 3.78232551E+01
 4
 C5H9Or_Olef_2m C 5 O 1 H 9 G 3E+02 1E+03 6E+02
 1
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 12 2
 -1.06183871E+04 1.03531661E+01 3.92002753E+00 4.06215381E-02-1.20784083E-
 05 3
 -7.27894915E-09 4.72684632E-12-1.06183871E+04 1.03531661E+01
 4
 C5H8_Olef C 5 H 8 G100.000 5000.000 1024.20
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 9.21486224E+00 2.55668049E-02-9.91978441E-06 1.82643604E-09-1.28318832E-
 13 2
 1.22947087E+04-2.13390042E+01 2.08099595E+00 3.35779126E-02 7.41938501E-
 06 3
 -2.83833715E-08 1.18648139E-11 1.47971249E+04 1.83309601E+01
 4
 C5H9Or_Olef_40 C 5 H 9 O 1 G100.000 5000.000 1532.69
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 1.10981550E+01 2.99930804E-02-1.25908831E-05 2.31433342E-09-1.58049661E-
 13 2
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 05 3
 1.29341403E-08-1.89026514E-12-1.21740220E+04 2.01760246E+01
 4
 C5H7Or_Olef C 5 H 7 O 1 G100.000 5000.000 1925.33
 1
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 13 2
 2.73787379E+04 1.30763977E+02 6.55178915E-01 5.12988196E-02-3.51579509E-
 05 3
 1.27778513E-08-2.22122898E-12 1.64758555E+04 2.68924785E+01
 4

C3H4O_Olef C 3 H 4 O 1 G100.000 5000.000 2012.21
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 13 2
 1.35286234E+04 1.31074213E+02 1.88376801E+00 3.08083513E-02-2.49083880E-
 05 3
 1.10214329E-08-2.13301049E-12 5.79454955E+02 1.57768931E+01
 4
 C4H6O_Olef_7 C 4 H 6 O 1 G100.000 5000.000 1648.60
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 13 2
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 05 3
 7.70180724E-09-1.03698622E-12-4.49601623E+03 1.55066595E+01
 4
 C5H7r_Olef C 5 H 7 G100.000 5000.000 1105.44
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 9.67790300E+00 2.20706668E-02-8.69621769E-06 1.59482662E-09-1.10865400E-
 13 2
 3.72031646E+04-2.14370959E+01 2.07558532E+00 3.66327897E-02-1.08884050E-
 05 3
 -7.67766073E-09 4.38213927E-12 3.96749865E+04 1.95797122E+01
 4
 C5H7r_Olef_1 C 5 H 7 G100.000 5000.000 973.64
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 9.77459243E+00 2.12806301E-02-7.49416350E-06 1.29741407E-09-8.80466703E-
 14 2
 2.87819445E+04-2.42401895E+01 1.92109642E+00 3.94948268E-02-1.39092626E-
 05 3
 -9.13125946E-09 6.39529981E-12 3.09772094E+04 1.68585816E+01
 4
 fulvene T12/10C 6.H 6. 0. 0.G 200.000 6000.000 1000.
 1
 1.14345282E+01 1.99371432E-02-7.13567060E-06 1.14951842E-09-6.87263886E-
 14 2
 2.04411455E+04-3.86799524E+01 5.09714763E-01 2.58195980E-02 5.06504954E-
 05 3
 -9.32593825E-08 4.15963672E-11 2.44318827E+04 2.30638077E+01
 2.60142888E+04 4
 CC(C)*CCJOH H 9C 50 1 0g 300.000 2500.0001000.000
 1
 0.68750448E+01 0.38884755E-01-0.19655206E-04 0.48873243E-08-0.48427549E-
 12 2
 -0.12811420E+05-0.65660262E+01 0.36941543E+01 0.38695809E-01 0.41729736E-
 05 3
 -0.30651517E-07 0.14599350E-10-0.11610798E+05 0.11757016E+02
 HHC 3 P 4
 C*(C)CJCOH H 9C 50 1 0g 300.000 2500.0001000.000
 1
 0.68988080E+01 0.38523566E-01-0.19368763E-04 0.48060089E-08-0.47660161E-
 12 2
 -0.89904463E+04-0.56711898E+01 0.20673068E+01 0.49566433E-01-0.20857377E-
 04 3
 -0.68589237E-08 0.64678562E-11-0.76568315E+04 0.19557276E+02
 HHC 3 P 4
 Prenol H 10C 50 1 0g 300.000 2500.0001000.000
 1

0.56371994E+01 0.42369727E-01-0.20979589E-04 0.50951972E-08-0.49203675E-
 12 2
 -0.26521791E+05 0.87928176E+00 0.75622902E+01 0.19993341E-01 0.39928498E-
 04 3
 -0.58570116E-07 0.22719885E-10-0.26287441E+05-0.50776429E+01
 HHC 4 P 4
 CC(CJ)*CC(*O) C 5 H 7 O 1 G100.000 5000.000 1608.84
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 -2.33199615E-01 4.49988713E-02-2.07326779E-05 3.25458329E-09-1.83687636E-
 13 2
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 05 3
 1.71935451E-08-3.12134765E-12-2.61831553E+03 2.20307476E+01
 4
 Ccy(CJCOC*C) C 5 H 7 O 1 G100.000 5000.000 901.43
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 9.62991454E+00 2.40793488E-02-8.15505606E-06 1.48128011E-09-1.08042333E-
 13 2
 -3.46860791E+03-2.89458147E+01 2.71044615E+00 5.74323675E-03 1.03960561E-
 04 3
 -1.41786564E-07 5.63628882E-11-2.28651749E+02 1.47702585E+01
 4
 Ccy(C*COC*C) C 5 H 6 O 1 G100.000 5000.000 920.70
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 13 2
 -1.28985517E+04-2.75137526E+01 2.37353776E+00 1.75501074E-02 6.00475762E-
 05 3
 -9.22527544E-08 3.73595935E-11-9.93313879E+03 1.66409146E+01
 4
 CC(C)*CCJ(*O) C 5 H 7 O 1 G100.000 5000.000 1117.17
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 7.68934309E+00 3.15945435E-02-1.49560866E-05 2.87526970E-09-2.00843571E-
 13 2
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 05 3
 2.04186994E-08-4.12676142E-12-5.38124314E+03 1.82245106E+01
 4
 C5H7O2r_Olef_4 C 5 O 2 H 7 G 3E+02 1E+03 6E+02
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 1.02523218E+01 7.18896216E-03 5.58262857E-05-7.07811066E-08 2.65033866E-
 11 2
 -7.99884220E+03-1.53318186E+01 1.02523218E+01 7.18896216E-03 5.58262857E-
 05 3
 -7.07811066E-08 2.65033866E-11-7.99884220E+03-1.53318186E+01
 4
 C5H6O2_Olef_3 C 5 O 2 H 6 G 3E+02 1E+03 6E+02
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 6.75355274E+00 1.49046355E-02 4.56088750E-05-6.56609835E-08 2.56469093E-
 11 2
 -2.89287290E+04 1.87404131E+00 6.75355274E+00 1.49046355E-02 4.56088750E-
 05 3
 -6.56609835E-08 2.56469093E-11-2.89287290E+04 1.87404131E+00
 4
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 1
 -1.38867475E-01 6.76381184E-02-2.69848444E-05-1.51784870E-08 1.20663210E-
 11 2

-1.57655055E+04 2.29354591E+01-1.38867475E-01 6.76381184E-02-2.69848444E-05 3
-1.51784870E-08 1.20663210E-11-1.57655055E+04 2.29354591E+01
4
C5H6O2_Olef C 5 O 2 H 6 G 3E+02 1E+03 6E+02
1
2.63200179E+00 4.13401140E-02-1.05903588E-05-1.44599790E-08 8.60780536E-12 2
-2.71039136E+04 1.89005738E+01 2.63200179E+00 4.13401140E-02-1.05903588E-05 3
-1.44599790E-08 8.60780536E-12-2.71039136E+04 1.89005738E+01
4
C5H7O2r_Olef C 5 O 2 H 7 G 3E+02 1E+03 6E+02
1
4.50012466E+00 4.74419961E-02-4.06774881E-05 2.69355279E-08-9.00612710E-12 2
-7.56748190E+03 1.10303583E+01 4.50012466E+00 4.74419961E-02-4.06774881E-05 3
2.69355279E-08-9.00612710E-12-7.56748190E+03 1.10303583E+01
4
C5H8O3_Olef_4 C 5 O 3 H 8 G 3E+02 1E+03 6E+02
1
3.10225933E-01 9.21500493E-02-1.30172321E-04 1.08599749E-07-3.72947244E-11 2
-2.52975884E+04 2.81114299E+01 3.10225933E-01 9.21500493E-02-1.30172321E-04 3
1.08599749E-07-3.72947244E-11-2.52975884E+04 2.81114299E+01
4
C6H11Or C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
4.25606394E+00 3.64145489E-02 3.01784271E-05-6.07059906E-08 2.57617624E-11 2
-1.20322739E+04 1.20426289E+01 4.25606394E+00 3.64145489E-02 3.01784271E-05 3
-6.07059906E-08 2.57617624E-11-1.20322739E+04 1.20426289E+01
4
C4H4O_Olef C 4 O 1 H 4 G 3E+02 1E+03 6E+02
1
-4.91672842E-01 5.16590686E-02-6.12678711E-05 4.19193424E-08-1.23030779E-11 2
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4.19193424E-08-1.23030779E-11 5.30142136E+03 2.67149334E+01
4
C5H9O2r_1 C 5 O 2 H 9 G 3E+02 1E+03 6E+02
1
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-3.28699743E+04 3.95437784E+01-2.30053399E+00 7.63210272E-02-6.32435689E-05 3
2.51064206E-08-2.84561934E-12-3.28699743E+04 3.95437784E+01
4
C4H6O2_Olef_1 C 4 O 2 H 6 G 3E+02 1E+03 6E+02
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-5.60276783E+00 1.05274453E-01-1.61921759E-04 1.30930954E-07-4.18987072E-11 2
-3.85516999E+04 4.70903149E+01-5.60276783E+00 1.05274453E-01-1.61921759E-04 3

1.30930954E-07-4.18987072E-11-3.85516999E+04 4.70903149E+01
 4
 C5H9O2r_2(m0) C 5 O 2 H 9 G 3E+02 1E+03 6E+02
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 13 2
 -3.34702648E+04 2.48746493E+01 3.63604722E-01 6.99886280E-02-5.33663953E-
 05 3
 1.55499907E-08 7.74408884E-13-3.34702648E+04 2.48746493E+01
 4
 B1E3M3J C 5 H 9 G 3E+02 1E+03 6E+02
 1
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 13 2
 1.01400000E+04 2.61300000E+01 2.75761999E-01 4.73200000E-02-2.32400000E-
 05 3
 2.58899999E-09 9.51700003E-13 1.01400000E+04 2.61300000E+01
 4
 CJCCCC C 5 H 11 G 3E+02 1E+03 6E+02
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 1.28684000E+00 5.06600000E-02-2.34500000E-05 1.63899999E-09 1.30500000E-
 12 2
 5.03700000E+03 2.32000000E+01 1.28684000E+00 5.06600000E-02-2.34500000E-
 05 3
 1.63899999E-09 1.30500000E-12 5.03700000E+03 2.32000000E+01
 4
 C5H11r_3 C 5 H 11 G 3E+02 1E+03 6E+02
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 2.37098908E+00 3.91024178E-02 9.07694917E-06-3.55783800E-08 1.63056111E-
 11 2
 2.39890333E+03 1.50487795E+01 2.37098908E+00 3.91024178E-02 9.07694917E-
 06 3
 -3.55783800E-08 1.63056111E-11 2.39890333E+03 1.50487795E+01
 4
 C6H13r C 6 H 13 G 3E+02 1E+03 6E+02
 1
 1.10546000E+00 6.04400000E-02-2.71000000E-05 1.11699999E-09 1.79500000E-
 12 2
 2.51300000E+02 2.60000000E+01 1.10546000E+00 6.04400000E-02-2.71000000E-
 05 3
 1.11699999E-09 1.79500000E-12 2.51300000E+02 2.60000000E+01
 4
 C6H13r_6 C 6 H 13 G 3E+02 1E+03 6E+02
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 11 2
 -1.74263544E+03 1.65144735E+01 1.13034239E+00 5.61329632E-02-3.37779244E-
 06 3
 -3.38938616E-08 1.76848636E-11-1.74263544E+03 1.65144735E+01
 4
 CCJCCC C 5 H 11 G 3E+02 1E+03 6E+02
 1
 1.09966000E+00 4.64900000E-02-1.36000000E-05-6.31100002E-09 3.47300000E-
 12 2
 3.79900000E+03 2.53300000E+01 1.09966000E+00 4.64900000E-02-1.36000000E-
 05 3
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 4

C6H13r_5 C 6 H 13 G 3E+02 1E+03 6E+02
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2.09102000E-01 5.95100000E-02-2.29600000E-05-2.48200003E-09 2.77900000E-
12 2
-6.00600000E+02 3.06300000E+01 2.09102000E-01 5.95100000E-02-2.29600000E-
05 3
-2.48200003E-09 2.77900000E-12-6.00600000E+02 3.06300000E+01
4
C6H13r_1 C 6 H 13 G 3E+02 1E+03 6E+02
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12 2
1.37900000E+03 3.29700000E+01-1.02702000E+00 7.52500000E-02-5.38600000E-
05 3
2.06500000E-08-3.26200000E-12 1.37900000E+03 3.29700000E+01
4
C5H11r_4 C 5 H 11 G 3E+02 1E+03 6E+02
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12 2
4.25900000E+03 2.82800000E+01-2.27110001E-01 5.95300000E-02-3.88000000E-
05 3
1.25900000E-08-1.48100000E-12 4.25900000E+03 2.82800000E+01
4
C6H13r_7 C 6 H 13 G 3E+02 1E+03 6E+02
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5.36238124E+00 2.71356679E-02 5.62792315E-05-8.62409986E-08 3.46760686E-
11 2
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05 3
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4
C6H13r_4 C 6 H 13 G 3E+02 1E+03 6E+02
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4.00683466E+00 4.11382945E-02 2.24386791E-05-5.31557678E-08 2.30596224E-
11 2
-7.31082582E+02 8.77575726E+00 4.00683466E+00 4.11382945E-02 2.24386791E-
05 3
-5.31557678E-08 2.30596224E-11-7.31082582E+02 8.77575726E+00
4
C5H11r_1 C 5 H 11 G 3E+02 1E+03 6E+02
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1.53395996E-02 5.80300000E-02-3.63100000E-05 1.08500000E-08-1.04700000E-
12 2
4.60800000E+03 2.80300000E+01 1.53395996E-02 5.80300000E-02-3.63100000E-
05 3
1.08500000E-08-1.04700000E-12 4.60800000E+03 2.80300000E+01
4
CCCJCC C 5 H 11 G 3E+02 1E+03 6E+02
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2.79539320E+00 3.91081536E-02-7.19297907E-07-1.70371295E-08 6.92014210E-
12 2
3.71000834E+03 1.46738146E+01 2.79539320E+00 3.91081536E-02-7.19297907E-
07 3
-1.70371295E-08 6.92014210E-12 3.71000834E+03 1.46738146E+01
4
C6H13r_8 C 6 H 13 G 3E+02 1E+03 6E+02
1

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 05 3
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 C5H11r C 5 H 11 G 3E+02 1E+03 6E+02
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 12 2
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 13 2
 2.68103723E+03-4.15571853E+01 9.97253423E-01 5.60101131E-02-2.07397071E-
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 HX15DE2V C 8 H 12 G 3E+02 1E+03 6E+02
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 05 3
 2.62539961E-09 4.69521420E-12 1.42710323E+04 2.79100070E+01
 4
 HX15DE2V5M C 9 H 14 G 3E+02 1E+03 6E+02
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 1.91682830E-08-6.27070009E-13 9.61051970E+03 2.89819249E+01
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 2.07164627E+04 3.68146263E+01-1.01613709E+00 1.08456801E-01-9.72399548E-
 05 3
 4.97913025E-08-1.06100434E-11 2.07164627E+04 3.68146263E+01
 4
 C9H13r_Olef C 9 H 13 G 3E+02 1E+03 6E+02
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 12 2
 2.43651299E+04 1.49515300E+01 3.12154725E+00 7.59872178E-02-3.91973498E-
 05 3
 -2.86546922E-10 5.76868153E-12 2.43651299E+04 1.49515300E+01
 4
 C7H13r_Olef C 7 H 13 G 3E+02 1E+03 6E+02
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 5.10300941E+00 4.36631337E-02 1.95971926E-05-5.03159805E-08 2.18542908E-
 11 2

1.10344502E+04 7.52299281E+00 5.10300941E+00 4.36631337E-02 1.95971926E-05
 3
 -5.03159805E-08 2.18542908E-11 1.10344502E+04 7.52299281E+00
 4
 C7H9r_Olef_1 C 7 H 9 G 3E+02 1E+03 6E+02
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 3
 3.57680257E-09 1.76420681E-13 1.12158185E+04 1.23067310E+01
 4
 C10H15r_Olef_3 C 10 H 15 G 3E+02 1E+03 6E+02
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 1.90852936E+00 9.40844522E-02-5.27779418E-05 3.40610203E-10 8.14785522E-12
 2
 3.24600319E+04 2.50599567E+01 1.90852936E+00 9.40844522E-02-5.27779418E-05
 3
 3.40610203E-10 8.14785522E-12 3.24600319E+04 2.50599567E+01
 4
 C6H9r_Olef_2 C 6 H 9 G 3E+02 1E+03 6E+02
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 2
 1.84300000E+04 3.58300000E+01-2.19946000E+00 6.64600000E-02-4.93600000E-05
 3
 1.89500000E-08-2.89300000E-12 1.84300000E+04 3.58300000E+01
 4
 C8H13r_Olef C 8 H 13 G 3E+02 1E+03 6E+02
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 2
 2.21403932E+04 1.71474537E+01 3.50391914E+00 6.21909549E-02-1.55215184E-05
 3
 -1.96929610E-08 1.18713175E-11 2.21403932E+04 1.71474537E+01
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 C*C(C)CCC*C C 7 H 12 G 3E+02 1E+03 6E+02
 1
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 2
 3.16508931E+03 1.93841585E+01 2.47064593E+00 5.49725457E-02-5.83266496E-06
 3
 -2.79976198E-08 1.46781875E-11 3.16508931E+03 1.93841585E+01
 4
 C10H15r_Olef_1 C 10 H 15 G 3E+02 1E+03 6E+02
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 1.80595336E+00 9.62355542E-02-6.54152410E-05 1.84039410E-08 3.52057666E-13
 2
 3.17168573E+04 2.56273442E+01 1.80595336E+00 9.62355542E-02-6.54152410E-05
 3
 1.84039410E-08 3.52057666E-13 3.17168573E+04 2.56273442E+01
 4
 C6H9r_Olef_4 C 6 H 9 G 3E+02 1E+03 6E+02
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 2
 2.37399951E+04-1.44846906E+00 6.53175779E-01-7.91670454E-03 1.20079687E-05
 3

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 4
 C6H8_Olef C 6 H 8 G 3E+02 1E+03 6E+02
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 C*CCCCJC C 6 H 11 G 3E+02 1E+03 6E+02
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 C6H11r_Olef_1 C 6 H 11 G 3E+02 1E+03 6E+02
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 C6H9r_Olef_5 C 6 H 9 G 3E+02 1E+03 6E+02
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 2.52423456E+04 4.38012897E+00-8.48665185E-01 6.03547871E-03-1.83499392E-
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 C10H15r_Olef C 10 H 15 G 3E+02 1E+03 6E+02
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 C6H7r_Olef C 6 H 7 G 3E+02 1E+03 6E+02
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 C9H15r_Olef_2 C 9 H 15 G 3E+02 1E+03 6E+02
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 1.75978009E+04 2.21632465E+01 2.63684285E+00 7.25233354E-02-1.33347524E-
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 C8H11r_Olef_1 C 8 H 11 G 3E+02 1E+03 6E+02
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 C8H11r_Olef C 8 H 11 G 3E+02 1E+03 6E+02
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 3.41014972E+00 5.95586045E-02-1.80274821E-05-1.68294303E-08 1.10909657E-
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 2.90256425E+04 1.49782244E+01 3.41014972E+00 5.95586045E-02-1.80274821E-
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 4
 C8H11r_Olef_6 C 8 H 11 G 3E+02 1E+03 6E+02
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-8.48665185E-01 6.03547871E-03-1.83499392E-05 1.68778750E-08-5.41551574E-
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 C7H11r_Olef_3 C 7 H 11 G 3E+02 1E+03 6E+02
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 C7H11r_Olef_1 C 7 H 11 G 3E+02 1E+03 6E+02
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 C9H15r_Olef_1 C 9 H 15 G 3E+02 1E+03 6E+02
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 C8H11r_Olef_3 C 8 H 11 G 3E+02 1E+03 6E+02
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 13 2
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 C7H11r_Olef_4 C 7 H 11 G 3E+02 1E+03 6E+02
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 11 2
 1.79196995E+04 4.66061635E+00 5.00923999E+00 4.10307833E-02 1.70912290E-
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 C9H13r_Olef_1 C 9 H 13 G 3E+02 1E+03 6E+02
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 12 2

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 C8H11r_Olef_4 C 8 H 11 G 3E+02 1E+03 6E+02
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 C7H9r_Olef C 7 H 9 G 3E+02 1E+03 6E+02
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 1.84293557E+04 1.05695812E+01-2.62265938E+00 1.52164983E-02-3.38636992E-
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 C7H11r_Olef C 7 H 11 G 3E+02 1E+03 6E+02
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 C6H7r_Olef_1 C 6 H 7 G 3E+02 1E+03 6E+02
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 06 3
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 4
 C6H9r_Olef C 6 H 9 G 3E+02 1E+03 6E+02
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 1.88357450E+00 4.95263704E-02-2.23106928E-05-3.65310622E-09 4.96417445E-
 12 2
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 C8H11r_Olef_2 C 8 H 11 G 3E+02 1E+03 6E+02
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 C6H9r_Olef_1 C 6 H 9 G 3E+02 1E+03 6E+02
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 C6H11r_Olef (m0) C 6 H 11 G 3E+02 1E+03 6E+02
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 06 3
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 4
 C9H15r_Olef C 9 H 15 G 3E+02 1E+03 6E+02
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 3.62454119E+00 7.15815459E-02-1.35831819E-05-2.84597099E-08 1.58856891E-
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 4
 C9H15r_Olef_4 C 9 H 15 G 3E+02 1E+03 6E+02
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 12 2
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 05 3
 7.92301567E-09 4.25376640E-12 2.00398705E+04 2.29494366E+01
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 C10H15r_Olef_2 C 10 H 15 G 3E+02 1E+03 6E+02
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 11 2
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 C9H13r_Olef_2 C 9 H 13 G 3E+02 1E+03 6E+02
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 C6H9r_Olef_3 C 6 H 9 G 3E+02 1E+03 6E+02
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 1.32149476E-08-1.98793416E-12 3.21973985E+04 2.14997989E+01
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 C6H11r_Olef_ (m1) C 6 H 11 G 3E+02 1E+03 6E+02
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 11 2
 1.64222829E+04 1.38327749E+01 2.99822217E+00 4.66609080E-02 3.47431210E-
 06 3
 -3.76181146E-08 1.87753491E-11 1.64222829E+04 1.38327749E+01
 4

C7H13r_Olef_3 C 7 H 13 G 3E+02 1E+03 6E+02
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11 2
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06 3
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C7H13r_Olef_1 C 7 H 13 G 3E+02 1E+03 6E+02
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4.09567197E+00 5.26126680E-02 2.50453079E-06-3.70673425E-08 1.80929308E-
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06 3
-3.70673425E-08 1.80929308E-11 1.25551445E+04 1.09751220E+01
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05 3
-4.78740248E-08 2.16047097E-11 1.00840347E+04 1.22893425E+01
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4.25278093E+04 2.46416539E+01 1.80126340E+00 7.00377957E-02-4.25016781E-
05 3
6.83560312E-09 2.81568434E-12 4.25278093E+04 2.46416539E+01
4
C8H9r_Olef C 8 H 9 G 3E+02 1E+03 6E+02
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13 2
1.12158185E+04 1.23067310E+01-2.97579855E+00 8.44734265E-03-1.02711630E-
05 3
3.57680257E-09 1.76420681E-13 1.12158185E+04 1.23067310E+01
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C9H15r_Olef_6 C 9 H 15 G 3E+02 1E+03 6E+02
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C* CJCC* C C 6 H 9 G 3E+02 1E+03 6E+02
1
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12 2
3.64297771E+04 2.89516469E+01 4.48582748E-01 5.64074288E-02-3.74503021E-
05 3
1.31522035E-08-2.16462986E-12 3.64297771E+04 2.89516469E+01
4
C8H13r_Olef_2 C 8 H 13 G 3E+02 1E+03 6E+02
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 11 2
 1.52084569E+04 1.30691194E+01 3.91314366E+00 5.51529327E-02 7.58668580E-
 06 3
 -4.50025932E-08 2.12079733E-11 1.52084569E+04 1.30691194E+01
 4
 C10H13r_Olef C 10 H 13 G 3E+02 1E+03 6E+02
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 12 2
 3.54710729E+04 2.45759908E+01 1.52245698E+00 9.45150390E-02-7.43160609E-
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 C8H13r_Olef_6 C 8 H 13 G 3E+02 1E+03 6E+02
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 4.30541421E+04 1.08131912E+02-1.19238438E+00 8.46822026E-02-7.08243488E-
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 1.54130140E-08-2.15536875E-12 2.30246795E+04 2.71777502E+01
 4
 C6H8_Olef_1 C 6 H 8 G100.000 5000.000 1916.09
 1
 -3.16515266E-01 4.31859750E-02-1.75814196E-05 2.55725316E-09-1.36483143E-
 13 2
 3.02712227E+04 3.68496828E+01 6.26815503E-01 5.30513713E-02-3.45691529E-
 05 3
 1.16912543E-08-1.74880711E-12 2.77372181E+04 2.60161302E+01
 4
 C4H4 C 4 H 4 G100.000 5000.000 2063.43
 1
 -1.89955325E+01 4.40977538E-02-1.34095094E-05 7.97935922E-11 9.00272317E-
 14 2

4.89297273E+04 1.43998447E+02 2.02896278E+00 2.83214314E-02-2.01000777E-
 05 3
 8.10836690E-09-1.59351611E-12 3.49352578E+04 1.44517236E+01
 4
 CC(C)*CCOJ H 9C 5O 1 0g 300.000 2500.0001000.000
 1
 0.41834340E+01 0.43056894E-01-0.22208003E-04 0.56049929E-08-0.56150668E-
 12 2
 0.65634570E+03 0.84264078E+01 0.39486442E+01 0.28418461E-01 0.28307981E-
 04 3
 -0.51954871E-07 0.21359274E-10 0.13775018E+04 0.13135149E+02
 HHC 3 P 4
 C*CCJ(C)OH C 4 H 7 O 1 G100.000 5000.000 827.21
 1
 5.76134347E+00 2.91606449E-02-1.28934022E-05 2.34961314E-09-1.58147366E-
 13 2
 -8.44729122E+03-1.53549857E+00 2.23392900E+00 3.50174877E-02-3.20447560E-
 06 3
 -2.18265224E-08 1.20949911E-11-7.48050935E+03 1.71293086E+01
 4
 CJC(OH)C(*O)C C 4 O 2 H 7 G 3E+02 1E+03 6E+02
 1
 -1.58683134E+00 6.85187695E-02-7.22426580E-05 4.09501909E-08-9.21224454E-
 12 2
 -2.56259050E+04 3.57482530E+01-1.58683134E+00 6.85187695E-02-7.22426580E-
 05 3
 4.09501909E-08-9.21224454E-12-2.56259050E+04 3.57482530E+01
 4
 CC(C)(OH)CCHO C 5 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 5.63602325E+00 3.54721173E-02 2.58812002E-05-5.91697535E-08 2.64338378E-
 11 2
 -5.25114280E+04 5.63815898E+00 5.63602325E+00 3.54721173E-02 2.58812002E-
 05 3
 -5.91697535E-08 2.64338378E-11-5.25114280E+04 5.63815898E+00
 4
 C5H9O3r_Olef_3 100515H 9C 5O 3 0g 300.000 2500.0001000.000
 1
 0.12643505E+02 0.39153218E-01-0.20539510E-04 0.53275975E-08-0.55237694E-
 12 2
 -0.26268777E+05-0.33543232E+02 0.30953233E+01 0.65977395E-01-0.41030813E-
 04 3
 0.30339837E-08 0.49591217E-11-0.23831145E+05 0.15221416E+02
 HHC 5 M 4
 C5H9O3r_Olef_7 100515H 9C 5O 3 0g 300.000 2500.0001000.000
 1
 0.12621253E+02 0.45201659E-01-0.26885453E-04 0.77272784E-08-0.86983703E-
 12 2
 -0.27213785E+05-0.39074417E+02-0.38791606E+01 0.10502743E+00-0.10785703E-
 03 3
 0.55346849E-07-0.10840902E-10-0.23546408E+05 0.42185997E+02
 HHC 5 P 4
 C5H9O3r_Olef_8 100515H 9C 5O 3 0g 300.000 2500.0001000.000
 1
 0.18091820E+02 0.29981082E-01-0.14400044E-04 0.34429934E-08-0.33183065E-
 12 2
 -0.22603449E+05-0.64139450E+02-0.11167502E+02 0.16384114E+00-0.24623307E-
 03 3

0.18281048E-06-0.52466292E-10-0.17411465E+05 0.73277695E+02
 HHC 5 P 4
 C5H9O3r_Olef_4 100515H 9C 50 3 0g 300.000 2500.0001000.000
 1
 0.17169176E+02 0.30252917E-01-0.13815658E-04 0.30433562E-08-0.26071791E-
 12 2
 -0.23588537E+05-0.57490231E+02-0.96959931E+00 0.88391423E-01-0.73785530E-
 04 3
 0.19190477E-07 0.35679569E-11-0.19331574E+05 0.33314880E+02
 HHC 5 M 4
 C5H11O2r 100515H 11C 50 2 0g 300.000 2500.0001000.000
 1
 0.11797722E+02 0.41264664E-01-0.20573782E-04 0.50303148E-08-0.48815986E-
 12 2
 -0.40941715E+05-0.30222160E+02 0.24970629E+01 0.52705497E-01 0.88601928E-
 05 3
 -0.53244506E-07 0.26218612E-10-0.37945445E+05 0.20614944E+02
 HHC 6 M 4
 C5H11O2r_2 100615H 11C 50 2 0g 300.000 2500.0001000.000
 1
 0.13329684E+02 0.37914854E-01-0.18159224E-04 0.42838448E-08-0.40310382E-
 12 2
 -0.40355727E+05-0.37409489E+02 0.33041332E+01 0.69691092E-01-0.50321181E-
 04 3
 0.12329064E-07 0.19659578E-11-0.37982762E+05 0.12875298E+02
 HHC 6 P 4
 C5H11O4r_1 100615H 11C 50 4 0g 300.000 2500.0001000.000
 1
 0.16954138E+02 0.55160549E-01-0.36010671E-04 0.11197197E-07-0.13435910E-
 11 2
 -0.61962098E+05-0.64302109E+02-0.12531058E+01 0.91389425E-01-0.34682816E-
 04 3
 -0.29197800E-07 0.19705102E-10-0.56422902E+05 0.32779087E+02
 HHC 7 M 4
 C5H11O4r_18 100615H 11C 50 4 0g 300.000 2500.0001000.000
 1
 0.16120373E+02 0.53664878E-01-0.33462449E-04 0.10027964E-07-0.11693792E-
 11 2
 -0.62284730E+05-0.57598274E+02 0.54303443E+00 0.86939059E-01-0.37790880E-
 04 3
 -0.20448748E-07 0.15942051E-10-0.57704781E+05 0.24777243E+02
 HHC 7 M 4
 C5H9O3r_Olef_10 100615H 9C 50 3 0g 300.000 2500.0001000.000
 1
 0.10570088E+02 0.43665316E-01-0.23326384E-04 0.61016205E-08-0.63444855E-
 12 2
 -0.24949971E+05-0.23491861E+02 0.33769717E+01 0.60438897E-01-0.27286516E-
 04 3
 -0.86235499E-08 0.84732759E-11-0.22963854E+05 0.14034371E+02
 HHC 4 P 4
 C5H9O3r_Olef_12 100615H 9C 50 3 0g 300.000 2500.0001000.000
 1
 0.20527092E+02 0.30340275E-01-0.16330257E-04 0.43589572E-08-0.46341056E-
 12 2
 -0.15771742E+05-0.80457939E+02 0.34469101E+01 0.46032868E-01 0.51668481E-
 04 3
 -0.11387677E-06 0.51169624E-10-0.99717783E+04 0.14339459E+02
 HHC 5 M 4

C5H11O4r_21 100615H 11C 50 4 0g 300.000 2500.0001000.000
1
0.16219776E+02 0.51492777E-01-0.31234613E-04 0.91463725E-08-0.10473549E-
11 2
-0.57496559E+05-0.54137054E+02 0.74235954E+01 0.52070394E-01 0.25357371E-
04 3
-0.72648660E-07 0.32378843E-10-0.54089660E+05-0.33403304E+01
HHC 8 M 4
C5H11O4r_13 100615H 11C 50 4 0g 300.000 2500.0001000.000
1
0.25255388E+02 0.27495956E-01-0.11312785E-04 0.22067606E-08-0.16221440E-
12 2
-0.52166102E+05-0.10057465E+03-0.10711363E+02 0.18661845E+00-0.27669308E-
03 3
0.19921595E-06-0.54944525E-10-0.45596324E+05 0.69468384E+02
HHC 7 M 4
C5H11O4r_3 100615H 11C 50 4 0g 300.000 2500.0001000.000
1
0.86628942E+01 0.70984527E-01-0.46687263E-04 0.14479086E-07-0.17266944E-
11 2
-0.50059699E+05-0.21548813E+02 0.15623845E+01 0.67772388E-01 0.49940008E-
05 3
-0.52499551E-07 0.23885524E-10-0.46957988E+05 0.20794439E+02
HHC 5 M 4
C5H11O4r_5 100615H 11C 50 4 0g 300.000 2500.0001000.000
1
0.70345716E+01 0.73844850E-01-0.48690050E-04 0.15104414E-07-0.17995124E-
11 2
-0.48853590E+05-0.11416442E+02 0.20610459E+01 0.71200237E-01-0.13365760E-
04 3
-0.29020450E-07 0.14620465E-10-0.46585301E+05 0.18525219E+02
HHC 5 M 4
C2H4O2 100615H 4C 20 2 0g 300.000 2500.0001000.000
1
0.82289076E+01 0.16209126E-01-0.93358149E-05 0.26254512E-08-0.29065595E-
12 2
-0.42774812E+05-0.18773869E+02 0.29176984E+01 0.11344400E-01 0.43536256E-
04 3
-0.69021098E-07 0.28663998E-10-0.40534559E+05 0.12986873E+02
HHC 2 P 4

END

REACTIONS

Isoprenol=IC4H8+CH2O	7.31E+05	1.676	34760	!	CBS-QB3
B1E3M3J+OH=Prenol	2.50E+13	0.00	0.00	!	
Estimated					
Prenol=H2O+B13DE2M	3.46E+02	2.756	56851	!	CBS-QB3
IC4H7+CH2OH=Isoprenol	1.00E+13	0.00	0.00	!	
Estimated					
H+Isoprenol=H2+C*C(C)CCJOH	8.52E+05	2.42	4190	!	CBS-QB3
H+Isoprenol=H2+C*C(C)CJCOH	7.90E+05	2.45	3500	!	CBS-QB3
H+Isoprenol=H2+C*C(CJ)CCOH	2.23E+06	2.30	4230	!	CBS-QB3
H+Prenol=H2+CC(C)*CCJOH	1.19E+09	1.58	2210	!	
CBS-QB3					

H+Prenol=H2+C*(C)CJCOH	3.50E+06	2.31	4300	!
CBS-QB3				
H+Prenol=H2+CC(C)*CCOJ	3.46E+06	2.09	10025	! CBS-QB3
CH3+Isoprenol=CH4+C*(C)CCJOH	1.63E+01	3.44	7435	! CBS-QB3
CH3+Isoprenol=CH4+C*(C)CJCOH	4.80E+00	3.62	5600	! CBS-QB3
CH3+Isoprenol=CH4+C*(C)CCOJ	3.60E+01	3.33	6942	! CBS-QB3
CH3+Prenol=CH4+C*(C)CJCOH	3.50E+01	3.37	6500	!
CBS-QB3				
CH3+Prenol=CH4+CC(C)*CCJOH	5.56E+02	3.01	4943	!
CBS-QB3				
CH3+Prenol=CH4+CC(C)*CCOJ	2.92E+02	2.94	7410	! CBS-QB3
B13DE2M+OH=C*(C)CJCOH	1.30E+04	2.55	-5800	! CBS-QB3
CC(C)*CCJOH=CC(C)*CC*O+H	6.40E+10	1.03	42800	! CBS-QB3
CC(C)*CCJOH=C*(C)CJCOH	2.30E+06	1.95	35600	!
CBS-QB3				
C5H10O2_2=CC(C)(OH)CCHO	2.78E+10	0.526	50099	! CBS-QB3
CC(C)(OH)CCHO=C2H3OH+CH3COCH3	2.13E+15	-0.865	34459	!
CBS-QB3				

!*****
!***Genesys***
!*****

IC3H7+C5H12O=C3H8+CC(C)CJCOH	3.48E12	0.000	16873.4	
C5H11O3r_40=C5H11O3r_42	2.91E12	-0.230	22298.7	
C5H11O3r_48=C5H10O2_23+OH	7.00E10	0.100	9330.6	
C5H11O5r_18=C4H9O4r+CH2O	6.00E13	0.220	14098.6	
CH2CHO+Prenol=CH3CHO+CC(C)*CCJOH	1.22E13	0.000	17375.3	
C5H9O3r_Olef_12=C4H7O2r_Olef+CH2O	9.00E13	0.220	14098.6	
C5H11O3r_26=C5H10O_Olef+HO2	5.77E9	0.930	29799.3	
NC3H7+C5H10O_Olef_2=C3H8+C5H9Or_Olef_4	3.26E12	0.000	18307.4	
C5H11O3r_16=C5H11O3r_19	2.91E12	-0.230	22298.7	
C2H5+Isoprenol=C2H6+C*(C)CCJOH	3.61E12	0.000	15487.2	
O2+C5H12O=HO2+CC(C)CCOJ	1.00E13	0.000	46932.5	
C4H9O4r=IC4KETIT+OH	1.80E15	0.000	1500.9	
CH3+C5H10O_Olef=CH4+CC(C)*CCJOH	5.50E12	0.000	10707.2	
C5H11O3r_26=C5H11O3r_30	6.18E7	1.000	21070.2	
IC4H7-I1+C5H12O=IC4H8+C5H11Or_1	2.31E13	0.000	12451.9	
C5H9O5r_Olef_18=C5H9O5r_Olef_13	2.91E12	-0.230	22298.7	
C3H5-T+C5H10O_Olef_2=C3H6+C5H9Or_Olef_4	2.23E13	0.000	13885.9	
C5H11O3r_4=C5H11O3r_10	1.41E9	0.510	17600.0	
C5H11O3r_37=C5H10O2_25+OH	4.56E8	1.290	9889.8	
C5H11O3r_30=C5H10O2_4+OH	7.00E10	0.100	9330.6	
C2H3OH+OH=CH2CHO+H2O	1.05E+13	0.00	5975	
CH2CHO+CC(C)CC*O=CH3CHO+C5H9Or_2	8.17E12	0.000	17590.4	
C3H3+C5H12O=C3H4-A+C5H11Or_13	4.9E13	0.000	25835.9	
O2+Isoprenol=HO2+C*(C)CCOJ	3.00E13	0.000	39297.3	
C5H11Or_1=C*CCCOH+CH3	7.68E13	0.000	30615.9	
O2+C5H11O3r_30=C5H11O5r_25	1.30E11	0.230	-1579.8	
DUP				
C5H7O3r_Olef_4=C5H6O3_Olef+H3	5.2E10	1.000	18548.8	
IC4H7-I1+CC(C)CC*O=IC4H8+CC(C)CC*O	1.31E13	0.000	8412.8	
C5H11O4r_6=C5H10O3_12+OH	2.28E8	1.290	9889.8	
C4H71-3+C5H12O=C4H8-2+C5H11Or_1	2.07E13	0.000	29516.5	
C*(C)CJCOH+HO2=C5H10O3_Olef_5	8.39E9	0.600	-2105.6	

DUP

C5H1103r_40=C5H1103r_46	1.76E9	0.780	21849.4
O2+Isoprenol=HO2+C*(C)CCJOH	2.00E13	0.000	47468.8
C5H1103r_6=C5H1002_2+OH	2.28E8	1.290	9889.8
IC4H7-I1+C5H120=IC4H8+CC(C)CJCOH	1.65E13	0.000	10157.5
O2+C5H1103r=C5H1105r_10	1.23E11	0.400	-800.6

DUP

O2+C5H903r_olef_10=C5H905r_olef_3	1.45E7	1.590	1080.3
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DUP

HO2+C5H120=H2O2+CC(C)CCJOH	2.46E-5	5.260	7480.7
C5H1103r_39=C5H1103r_36	4.66E7	1.400	28658.5
B1E3M3J+OH=C5H100_olef_2	2.50E+13	0.00	0.00
CH2CHO+Isoprenol=CH3CHO+C*(C)CCOH	5.64E12	0.000	19048.3
OH+Prenol=H2O+CC(C)*CCJOH	2.30E4	2.600	-2079.3
CH2CHO+C5H100_olef_2=CH3CHO+C5H90r_olef_4	2.08E13	0.000	22896.2
C5H80_olef_1+HOCHO=IC4H7CHO+HOCHO	2.81E-2	3.286	-4509.9

DUP

C4H71-3+Prenol=C4H8-1+C*(C)CJCOH	1.07E13	0.000	27508.9
C4H71-3+Prenol=C4H8-2+C*(C)CJCOH	8.29E12	0.000	26098.8
C5H110r_1=C3H6+PC2H4OH	5.52E13	0.000	28536.6
CH3O2+C5H100_olef=CH3O2H+C5H90r_olef_1	2.04E1	3.590	17160.2
C5H1104r_18=C5H1104r_13	2.91E12	-0.230	22298.7
C4H702r_4=C4H60_olef_5+OH	4.44E+11	0.000	7821
CCJ*CCOH=C3H4-P+CH2OH	7.19E13	0.000	26529.0
!C5H903r_olef_10=C5H80_olef_1+HO2	1.83E10	0.790	15099.6
C5H80_olef_1+HO2=C5H903r_olef_10	5.11E+02	2.78	11301.21
PC2H4OH+Prenol=C2H5OH+CC(C)*CCJOH	2.69E12	0.000	13455.7
IC4KETIT=C4H702r+OH	1.59E20	-1.500	42857.5
C5H1103r_2=Isoprenol+HO2	3.66E10	0.790	15099.6
CH3CHCHO+Isoprenol=C2H5CHO+C*(C)CCOH	1.01E13	0.000	22250.9
C*(C)COOH)CCOH=C*(C)COJ)CCOH+OH	1.59E20	-1.500	42857.5
C3H5-S+Prenol=C3H6+CC(C)*CCJOH	1.61E13	0.000	7361.2
CH2CHO+Isoprenol=CH3CHO+C*(C)CCJOH	1.63E13	0.000	19406.8
C5H1104r_13=IC4KETIT+CH2OH	6.00E13	0.220	14098.6
CH3O2+Isoprenol=CH3O2H+C*(C)CCOH	7.68E-2	4.400	13546.5
C5H1104r_3=C4H903r+CH2O	6.00E13	0.220	14098.6
C5H1105r_39=C5H1003_3+HO2	5.20E8	1.128	10630.7
C4H702r_6=CH3+CH3COCHO	6.00E13	0.220	14098.6
C4H71-3+C5H120=C4H8-2+CC(C)CJCOH	1.57E13	0.000	27222.1
IC4H7+C5H100_olef_2=IC4H8+C5H90r_olef_4	1.10E14	0.000	29946.7
O2+C*(C)CCJOH=C5H903r_olef	2.02E13	-0.310	-337.0

DUP

C5H1105r_39=C5H1004_12+OH	1.13E11	0.330	26698.7
IC4H9+CC(C)CC*O=IC4H10+C5H90r_2	7.39E11	0.000	12714.8
C5H903r_olef_7=C5H80_olef_1+HO2	1.73E10	0.930	29799.3
C5H1103r_4=C5H1103r_8	1.76E9	0.780	21849.4
C5H1104r_16=C5H1003_16+OH	4.56E8	1.290	9889.8
C5H1003=C5H902r+OH	1.59E20	-1.500	42857.5
C5H1103r_21=C5H1002_7+OH	9.16E15	-1.080	18438.9
IC3H7+Isoprenol=C3H8+C*(C)CJCOH	3.45E12	0.000	14077.1
C2H5+CC(C)CC*O=C2H6+C5H90r_21	1.80E12	0.000	13670.8
C5H1105r_29=C5H1004_8+OH	3.64E7	1.190	14999.6
O2+C5H100_olef=HO2+C5H90r_olef_1	3.00E13	0.000	52899.4
CH2CHO+C5H120=CH3CHO+C5H110r_1	1.61E13	0.000	22466.0
C4H71-3+Isoprenol=C4H8-1+C*(C)CCOH	1.02E13	0.000	27508.9
C5H1103r_39=C5H1103r_48	6.18E7	1.000	21070.2
C5H1105r_6=C5H1105r_20	2.91E12	-0.230	22298.7
C3H3+Prenol=C3H4-A+CC(C)*CCJOH	1.90E13	0.000	20745.2

O2+C5H11O3r_9=C5H11O5r_6 7.54E14 -0.920 -129.1
DUP
C5H8O_olef_1=IC4H7CHO 4.42E42 -9.090 67068.2
C5H11O3r_16=C5H11O3r_21 1.76E9 0.780 21849.4
C5H9O2r_olef_4=C3H5-T+C2H4O28.10E14 0.000 23890.4
C5H9O2r_olef_7=CH3+C4H6O2_olef 1.20E14 0.220 14098.6
C2H3+CC(C)CC*O=C2H4+CCJ(C)CC*O 1.31E13 0.000 8412.8
!C5H9O5r_olef_3=C5H8O3_olef+HO2 7.80E8 1.128 10630.7
C5H9O5r_olef_3=C5H8O3_olef+HO2 1.20E+12 0.20 9800
C5H9Or_olef_1=C3H6+C2H2OH 4.19E13 0.000 33149.3
C5H11O5r_37=C5H11O5r_32 2.91E12 -0.230 22298.7
B13DE2MJ+IC4H7=HX15DE2V5M 1.00E+13 0.00 0.00
O2+C5H11O3r_9=C5H11O5r_6 7.54E14 -0.920 -129.1
DUP
!C5H9O3r_olef_10=C5H8O2_olef_8+OH 3.50E10 0.100 9330.6
O2+C5H9O3r_olef_10=C5H9O5r_olef_3 1.45E7 1.590 1080.3
DUP
C3H5-S+Isoprenol=C3H6+C*(C)CCJOH 2.16E13 0.000 9392.7
C3H3+C5H12O=C3H4-P+CCJ(C)CCOH 5.62E12 0.000 21366.6
C5H11O5r_16=C5H10O4+OH 4.23E9 0.510 17600.0
C4H71-3+C5H100_olef=C4H8-2+C5H9Or_olef_1 2.69E13 0.000 29946.7
C5H8O4_olef_2=C5H7O3r_olef_1+OH 1.59E20 -1.500 42857.5
NC3H7+Isoprenol=C3H8+C*(C)CCOH 8.25E11 0.000 14459.5
C4H71-3+C5H12O=C4H8-1+CCJ(C)CCOH 1.23E13 0.000 26457.3
O2+C5H11O3r_10=C5H11O5r_16 2.02E13 -0.310 -337.0
DUP
NC4KET23=C4H7O2r_6+OH 1.59E20 -1.500 42857.5
C3H5-S+C5H12O=C3H6+C5H11Or_12.31E13 0.000 12451.9
!C5H9O3r_olef_3=CC(C)*CC*O+HO2 5.20E8 1.128 10630.7
C5H9O3r_olef_3=CC(C)*CC*O+HO2 1.20E+12 0.20 9800
C5H11O5r_42=C5H10O4_14+OH 5.46E7 1.190 14999.6
C5H11O3r_26=CC(C)CC*O+HO2 5.20E8 1.128 10630.7
NC3H7+C5H12O=C3H8+C5H11Or_1 2.52E12 0.000 17877.2
NC3H7+Isoprenol=C3H8+C*(C)CCJOH 2.39E12 0.000 14818.0
CH3+CC(C)*CC*O=CH4+CC(C)*CCJ(*) 5.00E0 3.600 4328.3
C5H11O4r_18=C5H10O2_olef_3+HO2 2.88E9 0.930 29799.3
IC4H7+C5H100_olef=IC4H8+CC(C)*CCJOH 2.37E13 0.000 22967.9
HO2+CC(C)*CC*O=H2O2+CC(C)*CCJ(*) 1.18E-4 4.900 3680.6
H+C5H12O=H2+CC(C)CCJOH 4.16E13 0.000 10324.8
O2+C5H11O2r_2=C5H11O4r_1 7.54E14 -0.920 -129.1
DUP
IC3H7+Isoprenol=C3H8+C*(C)CCJOH 4.63E12 0.000 16108.6
C5H7O2r_olef_1=C4H5Or_olef_1+CH2O 8.10E14 0.000 23890.4
C2H3+Isoprenol=C2H4+C*(C)CCJOH 2.16E13 0.000 9392.7
C4H71-4+C5H100_olef_2=C4H8-1+C5H9Or_olef_4 4.94E12 0.000 18976.6
C2H3+C5H12O=C2H4+CC(C)CJCOH 1.65E13 0.000 10157.5
HO2+C5H100_olef=H2O2+C5H9Or_olef_1 2.04E1 3.590 17160.2
CH2CHO+C5H12O=CH3CHO+CC(C)CCJOH 1.25E13 0.000 18976.6
C5H11O3r_4=C5H11O3r 5.63E10 0.330 26698.7
PC2H4OH+C5H12O=C2H5OH+CC(C)CCJOH 2.75E12 0.000 15057.0
C5H9O2r_olef_7=CH3COCH3+C2H2OH 5.40E14 0.000 23890.4
C*CCOH=C3H6+CH2O 7.31E5 1.676 34760.2
C5H100_olef+HO2=CC(C)CC*O+HO2 9.92E4 1.670 6809.1
DUP
C5H11O4r_1=C5H11O4r_6 4.66E7 1.400 28658.5
CC(C)CC*O+H=CC(C)CCJOH 2.20E14 0.000 10700.0
OH+Prenol=H2O+CC(C)*CCOJ 2.30E+03 2.90 621
O2+C5H9O3r_olef_13=C5H9O5r_olef_18 1.45E7 1.590 1080.3

DUP
C2H3+C5H12O=C2H4+CCJ(C)CCOH 9.99E12 0.000 7982.6
C5H10O4_12=C5H9O3r_11+OH 1.59E20 -1.500 42857.5
O2+C*C(C)CJCOH=C5H9O3r_Olef_8 1.45E7 1.590 1080.3
DUP
C5H11O3r_5=C5H11O3r_2 7.68E12 -0.130 34358.6
C5H7O3r_Olef_1=C4H5Or_Olef+HOCHO 8.10E14 0.000 23890.4
C5H11O3r_36=C5H10O_Olef_2+HO2 1.83E10 0.790 15099.6
H+CC(C)CC*O=H2+CCJ(C)CC*O 1.11E14 0.000 7576.3
C3H3+Isoprenol=C3H4-P+C*C(C)CJCOH 9.49E12 0.000 20745.2
C5H11O5r_37=C5H10O4_10+OH 1.13E11 0.330 26698.7
O2+C5H11O3r_25=C5H11O5r_37 7.54E14 -0.920 -129.1
DUP
C3H5-A+C5H12O=C3H6+CC(C)CJCOH 3.17E13 0.000 27222.1
C5H9O3r_4=CH3+C4H6O3 9.00E13 0.220 14098.6
O2+C*C(C)CJCOH=C5H9O3r_Olef_4 1.45E7 1.590 1080.3
DUP
C5H9O5r_Olef_9=C5H8O4_Olef_4+OH 1.34E7 1.290 14239.6
IC4H7+Isoprenol=IC4H8+C*C(C)CJCOH 7.15E13 0.000 24425.8
C5H11O5r_32=C4H9O2r+HO2CHO 6.00E13 0.220 14098.6
C5H10O3_Olef_5=C5H9O2r_Olef_3+OH 1.59E20 -1.500 42857.5
C5H11O5r_9=C5H11O5r_18 2.91E12 -0.230 22298.7
C3H5-T+Isoprenol=C3H6+C*C(C)CJCOH 1.19E13 0.000 8365.0
C2H5+Isoprenol=C2H6+C*C(C)CJCOH 2.69E12 0.000 13455.7
CH3O2+CC(C)CC*O=CH3O2H+C5H9Or 2.04E1 3.590 17160.2
O2+C*C(CJ)CCOH=C*C(COOJ)CCOH 5.80E7 1.590 1080.3
C5H11O3r_19=C4H9O2r+CH2O 6.00E13 0.220 14098.6
C3H5-T+Isoprenol=C3H6+C*C(CJ)CCOH 5.53E12 0.000 10038.0
C5H9O3r_7=C4H7O2r_3+CH2O 9.00E13 0.220 14098.6
C5H9O3r_Olef_13=C5H8O2_Olef_8+OH 3.50E10 0.100 9330.6
CC(C)CCJ(*O)=IC4H9+CO 3.30E12 0.620 17298.8
CH3+C5H10O_Olef=CH4+C5H9Or_Olef_1 3.10E13 0.000 17686.0
C5H11O3r_37=C5H10O_Olef_2+HO2 3.66E10 0.790 15099.6
C5H10O3_3=C5H9O2r_3+OH 1.59E20 -1.500 42857.5
C5H9O3r_Olef_13=C5H8O_Olef_1+HO2 1.83E10 0.790 15099.6
PC2H4OH+C5H10O_Olef=C2H5OH+CC(C)*CCJOH 8.92E11 0.000 11997.8
C3H5-S+Isoprenol=C3H6+C*C(C)CJCOH 1.61E13 0.000 7361.2
O2+C5H11O3r_8=C5H11O5r_2 1.30E11 0.230 -1579.8
DUP
C5H10O3_Olef_6=C5H9O2r_Olef_1+OH 1.59E20 -1.500 42857.5
C3H3+Isoprenol=C3H4-A+C*C(CJ)CCOH 4.40E12 0.000 22418.2
O2+C5H11O3r_30=C5H11O5r_25 1.30E11 0.230 -1579.8
DUP
PC2H4OH+CC(C)CC*O=C2H5OH+C5H9Or 3.86E12 0.000 18546.4
CH3CHCHO+CC(C)CC*O=C2H5CHO+C5H9Or_2 1.46E13 0.000 20793.0
C5H11O4r_18=C5H11O4r_16 7.68E12 -0.130 34358.6
IC4H7+C5H10O_Olef=IC4H8+C5H9Or_Olef_1 1.12E14 0.000 29946.7
IIC4H7Q2-I=IC4KETII+OH 2.70E15 0.000 1500.9
C5H10O3_2=C5H9O2r_2+OH 1.59E20 -1.500 42857.5
C5H11O3r_42=NC4KET23+CH3 1.20E14 0.220 14098.6
H+CC(C)CC*O=H2+C5H9Or_2 1.63E14 0.000 9082.0
C5H11O3r_23=C5H10O_Olef+HO2 1.83E10 0.790 15099.6
C5H9O3r_Olef=C5H8O_Olef_1+HO2 5.77E9 0.930 29799.3
IC4KETII=CHOIC3H6O+OH 1.59E20 -1.500 42857.5
C3H3+Isoprenol=C3H4-P+C*C(C)CCJOH 1.21E13 0.000 22776.7
C5H8O_Olef_1+HO2=IC4H7CHO+HO2 1.49E5 1.670 6809.1
DUP
C4H71-4+Isoprenol=C4H8-1+C*C(CJ)CCOH 1.25E12 0.000 15128.7

C5H9O3r_Olef_3=C5H9O3r_Olef_13 6.72E6 1.290 14239.6
CH2OH+Prenol=CH3OH+C*(C)CJCOH 5.66E12 0.000 18331.3
C5H11O3r_25=C5H10O_Olef+HO2 1.83E10 0.790 15099.6
C4H71-3+CC(C)CC*O=C4H8-1+CCJ(C)CC*O 1.61E13 0.000 26887.5
O2+C5H11O3r_2=C5H11O5r_3 1.30E11 0.230 -1579.8
DUP
OH+CC(C)CC*O=H2O+CC(C)CCJ(*O) 6.13E4 2.700 -4588.8
O2+C5H12O=HO2+CC(C)CCJOH 2.00E13 0.000 47468.8
C5H10O_Olef+HO2=CC(C)CC*O+HO2 9.92E4 1.670 6809.1
DUP
C3H5-S+C5H10O_Olef_2=C3H6+C5H9Or_Olef_4 3.01E13 0.000 12882.1
O2+C5H11O2r_2=C5H11O4r_1 7.54E14 -0.920 -129.1
DUP
H+C5H12O=H2+CCJ(C)CCOH 1.11E14 0.000 7576.3
C4H71-3+C5H10O_Olef=C4H8-1+C5H9Or_Olef_1 3.36E13 0.000 31356.8
O2+CC(C)CCJOH=C5H11O3r_26 2.02E13 -0.310 -337.0
DUP
H+C5H10O_Olef_2=H2+C5H9Or_Olef_4 3.51E14 0.000 12786.5
C5H9O3r_13=C4H7O2r_4+CH2O 9.00E13 0.220 14098.6
O2+C5H11O3r_10=C5H11O5r_16 2.02E13 -0.310 -337.0
DUP
O2+C*(C)CCJOH=C5H9O3r_Olef 2.02E13 -0.310 -337.0
DUP
NC3H7+CC(C)CC*O=C3H8+C5H9Or 2.52E12 0.000 17877.2
C3H5-T+C5H12O=C3H6+CC(C)CCJOH 1.22E13 0.000 9966.3
O2+CC(C)CJCOH=C5H11O3r_16 7.54E14 -0.920 -129.1
DUP
C3H5-T+CC(C)CC*O=C3H6+C5H9Or_2 8.01E12 0.000 8580.1
C5H10O4=C5H9O3r+OH 1.59E20 -1.500 42857.5
C5H11O3r_26=C5H11O3r_28 1.82E7 1.190 14999.6
C5H11O3r_5=Isoprenol+HO2 1.73E10 0.930 29799.3
C4H71-3+CC(C)CC*O=C4H8-2+CCJ(C)CC*O 1.30E13 0.000 25477.4
PC2H4OH+CC(C)CC*O=C2H5OH+C5H9Or_2 1.80E12 0.000 13670.8
C*(C)CJCOH+HO2=C5H10O3_Olef_5 8.39E9 0.600 -2105.6
DUP
C2H5+Isoprenol=C2H6+C*(C)CJCOH 1.25E12 0.000 15128.7
C5H11O2r_2=C5H10O_Olef_2+OH 3.00E13 0.000 26799.1
C5H11O3r_23=C5H10O2_18+OH 2.28E8 1.290 9889.8
C5H11O5r_47=C5H10O4_15+OH 1.13E11 0.330 26698.7
C5H11O4r_1=C5H11O4r_5 2.91E12 -0.230 22298.7
C5H10O_Olef=CC(C)CC*O 2.95E42 -9.090 67068.2
IC4H7+C5H12O=IC4H8+CC(C)CJCOH 6.45E13 0.000 27222.1
C2H3+Isoprenol=C2H4+C*(C)CJCOH 1.61E13 0.000 7361.2
C2H3+C5H10O_Olef=C2H4+CC(C)*CCJOH 5.34E12 0.000 5903.3
O2+C*(C)CJCOH=C5H9O3r_Olef_4 1.45E7 1.590 1080.3
DUP
C5H9Or_Olef_4=C2H3+IC3H5OH 7.61E13 0.000 35754.4
C3H5-T+Prenol=C3H6+C*(C)CJCOH 5.53E12 0.000 10038.0
C2H5+C5H12O=C2H6+CC(C)CCJOH 2.75E12 0.000 15057.0
C3H3+C5H10O_Olef=C3H4-P+C5H9Or_Olef_1 1.55E13 0.000 26266.1
CH2CHO+C5H12O=CH3CHO+CCJ(C)CCOH 7.56E12 0.000 17996.7
O2+C5H11O3r_7=C5H11O5r_13 2.02E13 -0.310 -337.0
DUP
IC4H9+C5H10O_Olef=IC4H10+C5H9Or_Olef_1 2.05E12 0.000 18020.6
C5H9O5r_Olef_13=C4H7O2r_Olef+HO2CHO 9.00E13 0.220 14098.6
O2+C5H11O3r_15=C5H11O5r_47 2.46E11 0.400 -800.6
DUP
CC(C)*CCJOH+HO2=C5H10O3_Olef_1 8.39E9 0.600 -2105.6

DUP

C5H9O3r_Olef_8=C5H9O3r_Olef_10 4.48E6 1.290 14239.6
C5H11O4r_6=C5H10O2_Olef+HO2 1.83E10 0.790 15099.6
C5H11O3r_42=C2H5O2r+CH3COCH3 6.00E13 0.220 14098.6
CCJ(C)CCOH=IC4H8+CH2OH 7.19E13 0.000 26529.0
C5H9O2r_3=IC3H7+CHOCHO 6.00E13 0.220 14098.6
IC4H7-I1+C5H10O_Olef=IC4H8+CC(C)*CCJOH 5.34E12 0.000 5903.3
O2+C5H9O3r_Olef_13=C5H9O5r_Olef_9 1.45E7 1.590 1080.3

DUP

CH3+CC(C)CC*O=CH4+CCJ(C)CC*O 1.35E13 0.000 13216.7
C3H5-A+C5H12O=C3H6+CCJ(C)CCOH 2.00E13 0.000 25047.2
C5H9O3r_4=CH3COCHO+PC2H4OH 9.00E13 0.220 14098.6
C5H9O2r_2=CH3+C4H6O2 1.20E14 0.220 14098.6
NC3H7+Prenol=C3H8+CC(C)*CCJOH 1.78E12 0.000 12786.5
O2+C5H9O3r_Olef_10=C5H9O5r_Olef_7 1.45E7 1.590 1080.3

DUP

CH2CHO+C5H12O=CH3CHO+CC(C)CJCOH 1.21E13 0.000 20171.6
CH3+CC(C)CC*O=CH4+C5H9Or 2.38E13 0.000 17255.8
CC(C)CCJ(*O)=IC3H7+CH2CO 7.04E13 0.000 30711.5
HO2+C5H10O_Olef=H2O2+CC(C)*CCJOH 2.56E-2 4.400 13546.5
C5H9O3r_Olef_4=C5H9O3r_Olef_12 2.91E12 -0.230 22298.7
CH2OH+CC(C)CC*O=CH3OH+C5H9Or 1.63E13 0.000 21749.0
C3H5-T+Prenol=C3H6+CC(C)*CCJOH 1.19E13 0.000 8365.0
O2+C*C(C)CJCOH=C5H9O3r_Olef_8 1.45E7 1.590 1080.3

DUP

C3H5-S+CC(C)CC*O=C3H6+C5H9Or 2.31E13 0.000 12451.9
C5H8O_Olef_1+HO2=IC4H7CHO+HO2 1.49E5 1.670 6809.1

DUP

C*C(C)CJCOH+HO2=C5H10O3_Olef_2 8.39E9 0.600 -2105.6

DUP

C4H71-3+Prenol=C4H8-1+CC(C)*CCJOH 2.31E13 0.000 25835.9
C4H71-3+C5H10O_Olef_2=C4H8-1+C5H9Or_Olef_4 3.29E13 0.000 31356.8
C2H5+CC(C)CC*O=C2H6+C5H9Or 3.78E12 0.000 18546.4
C5H8O3_Olef=C5H7O2r_Olef_1+OH 1.59E20 -1.500 42857.5
C5H10O4_15=C5H9O3r_15+OH 1.59E20 -1.500 42857.5
IC4H9+Isoprenol=IC4H10+C*C(C)CCJOH 1.48E12 0.000 14531.2
C5H11O3r_16=C5H11O3r_15 5.63E10 0.330 26698.7
C5H11O3r_16=Prenol+HO2 2.88E9 0.930 29799.3
CH2CHO+CC(C)CC*O=CH3CHO+CCJ(C)CC*O 9.92E12 0.000 18426.9
C4H71-4+C5H10O_Olef=C4H8-1+CC(C)*CCJOH 8.92E11 0.000 11997.8
H+C5H12O=H2+C5H11Or_1 3.36E14 0.000 12595.3
C*C(C)CCJOH=C3H5-T+C2H3OH 3.07E14 0.000 35300.3
CH2OH+CC(C)CC*O=CH3OH+C5H9Or_2 8.19E12 0.000 16873.4
C5H9O2r_Olef_4=IC3H5CHO+CH2OH 9.00E13 0.220 14098.6
C5H10O4_7=C5H9O3r_7+OH 1.59E20 -1.500 42857.5
C2H5+C5H10O_Olef_2=C2H6+C5H9Or_Olef_4 4.89E12 0.000 18976.6
CH3+C5H10O_Olef_2=CH4+C5H9Or_Olef_4 3.10E13 0.000 17686.0
C5H9O2r_Olef_3=CCJ*CCOH+CH2O 8.10E14 0.000 23890.4
C5H11O3r_4=C5H11O3r_9 1.64E11 0.130 19468.9
C5H11O4r_16=C5H10O2_Olef_2+HO2 3.66E10 0.790 15099.6
C5H10O4_10=C5H9O3r_10+OH 1.59E20 -1.500 42857.5
C3H5-A+C5H12O=C3H6+CC(C)CCJOH 3.28E13 0.000 26027.1
C3H5-A+CC(C)CC*O=C3H6+CCJ(C)CC*O 2.63E13 0.000 25477.4
O2+CC(C)*CCJOH=C5H9O3r_Olef_3 1.45E7 1.590 1080.3

DUP

C5H11O3r_26=C5H11O3r_25 4.66E7 1.400 28658.5
CH2OH+C5H10O_Olef_2=CH3OH+C5H9Or_Olef_4 2.11E13 0.000 22179.2
IC4H7+Prenol=IC4H8+CC(C)*CCJOH 7.15E13 0.000 24425.8

O2+CC(C)CC*O=HO2+C5H9Or 3.00E13 0.000 53567.7
IC4H7-I1+CC(C)CC*O=IC4H8+C5H9Or 2.31E13 0.000 12451.9
OH+CC(C)CC*O=H2O+C5H9Or 1.67E6 2.078 375.3
IC4H9+Isoprenol=IC4H10+C*C(CJ)CCOH 5.10E11 0.000 14172.7
C5H8O_olef_1+HOCHO=IC4H7CHO+HOCHO 2.81E-2 3.286 -4509.9
DUP
C2H3+C5H10O_olef_2=C2H4+C5H9Or_olef_4 3.01E13 0.000 12882.1
CH2OH+CC(C)CC*O=CH3OH+CCJ(C)CC*O 9.94E12 0.000 17709.9
C5H11O3r_2=C5H10O2_13+OH 4.56E8 1.290 9889.8
CH2OH+C5H10O_olef=CH3OH+C5H9Or_olef_1 2.15E13 0.000 22179.2
C4H71-3+Isoprenol=C4H8-1+C*C(C)CCJOH 2.63E13 0.000 27867.4
C3H5-A+C5H10O_olef=C3H6+C5H9Or_olef_1 5.52E13 0.000 29946.7
CH3CHCHO+C5H10O_olef=C2H5CHO+CC(C)*CCJOH 7.20E12 0.000 19120.0
CH2CHO+C5H10O_olef=CH3CHO+CC(C)*CCJOH 4.04E12 0.000 15917.4
C3H5-A+Isoprenol=C3H6+C*C(C)CCJOH 4.30E13 0.000 26457.3
C5H11O3r_46=C5H10O2_21+OH 9.16E15 -1.080 18438.9
C5H9O3r_olef_13=C5H8O2_olef_13+OH 2.28E8 1.290 9889.8
C*C(C)CCJOH=C*C(CJ)CCOH 9.00E11 0.000 26218.3
O2+C5H11O3r=C5H11O5r_10 1.23E11 0.400 -800.6
DUP
CC(C)*CCJOH+HO2=C5H10O3_olef_1 8.39E9 0.600 -2105.6
DUP
C5H9O2r_olef_3=C5H8O2_olef_1+H 3.52E10 1.000 18548.8
IC3H7+Isoprenol=C3H8+C*C(CJ)CCOH 1.60E12 0.000 15750.1
C4H71-3+C5H12O=C4H8-1+CC(C)CJCOH 1.94E13 0.000 28632.2
C5H11O5r_10=C5H10O4_5+OH 1.40E8 1.400 28658.5
C5H9O5r_olef_3=C5H8O4_olef_2+OH 2.68E7 1.290 14239.6
C2H3+CC(C)CC*O=C2H4+C5H9Or 2.31E13 0.000 12451.9
CCJ(C)CC*O=IC4H8+HCO 5.59E13 0.000 23923.9
C5H11O4r_1=C5H11O4r_7 1.76E9 0.780 21849.4
HO2+C5H12O=H2O2+C5H11Or_1 2.04E1 3.590 17160.2
C*C(COJ)CCOH=C*C(C*O)CCOH+H 1.17E10 1.000 18548.8
IC3H7+C5H10O_olef_2=C3H8+C5H9Or_olef_4 5.99E12 0.000 19598.0
C4H71-3+Isoprenol=C4H8-2+C*C(C)CJCOH 1.79E13 0.000 24425.8
IC4H7+C5H12O=IC4H8+CC(C)CCJOH 6.66E13 0.000 26027.1
C5H9Or_olef_1=C4H6O_olef_4+CH3 4.26E13 0.000 27317.7
C*C(CJ)CCOH=C3H4-A+PC2H4OH 3.11E15 0.000 56595.2
OH+C5H12O=H2O+CC(C)CJCOH 5.42E12 0.000 1576.8
C2H5+C5H10O_olef=C2H6+C5H9Or_olef_1 4.97E12 0.000 18976.6
IC4H7+Isoprenol=IC4H8+C*C(C)CCJOH 8.74E13 0.000 26457.3
O2+C5H11O3r_28=C5H11O5r_29 2.46E11 0.400 -800.6
DUP
C3H3+C5H10O_olef=C3H4-A+C5H9Or_olef_1 4.60E13 0.000 26266.1
C5H7O2r_olef_1=C5H6O2_olef_1+H 3.52E10 1.000 18548.8
O2+C5H10O_olef=HO2+CC(C)*CCJOH 1.00E13 0.000 31230.9
O2+CC(C)*CCJOH=C5H9O3r_olef_3 1.45E7 1.590 1080.3
DUP
O2+C5H11O3r_28=C5H11O5r_29 2.46E11 0.400 -800.6
DUP
C3H5-S+CC(C)CC*O=C3H6+C5H9Or_2 1.08E13 0.000 7576.3
C5H11O4r_18=C5H10O2_olef_2+HO2 1.73E10 0.930 29799.3
H+CC(C)*CC*O=H2+CC(C)*CCJ(*O) 7.15E5 2.400 1577.4
C*CCJ(C)OH+OH=C4H8O2_olef_1 2.50E+13 0.00 0.00
CH2OH+Isoprenol=CH3OH+C*C(CJ)CCOH 5.66E12 0.000 18331.3
C4H71-3+CC(C)CC*O=C4H8-1+C5H9Or 2.55E13 0.000 30926.6
O2+Prenol=HO2+CC(C)*CCJOH 2.00E13 0.000 31371.1
O2+CC(C)CJCOH=C5H11O3r_16 7.54E14 -0.920 -129.1
DUP

CH3CHCHO+C5H10O_olef_2=C2H5CHO+C5H9Or_olef_4 3.45E13 0.000 26098.8
 PC2H4OH+C5H12O=C2H5OH+CCJ(C)CCOH 1.67E12 0.000 14077.1
 IC3H7+CC(C)CC*O=C3H8+CCJ(C)CC*O 2.81E12 0.000 15128.7
 O2+C5H9O3r_olef_10=C5H9O5r_olef_7 1.45E7 1.590 1080.3
 DUP
 Prenol+OH=C5H11O2r_2 7.80E7 1.290 -2652.9
 C5H9Or_2=CH3+CH3CHCHCHO 3.17E14 0.000 35515.4
 IC4H9+C5H12O=IC4H10+C5H11Or_1 1.56E12 0.000 17590.4
 !C5H9O3r_olef_10=C5H8O2_olef_5+OH 2.28E8 1.290 9889.8
 C5H9O3r_8=CH3+C4H6O3_1 1.20E14 0.220 14098.6
 C5H11O5r_13=C5H10O3_2+HO2 5.20E8 1.128 10630.7
 C5H11O3r_6=Prenol+HO2 1.83E10 0.790 15099.6
 B13DE2MJ+C3H5-A=HX15DE2V 1.00E+13 0.00 0.00
 C3H5-S+C5H10O_olef=C3H6+C5H9Or_olef_1 3.01E13 0.000 12882.1
 HO2+Prenol=H2O2+CC(C)*CCJOH 2.7E-01 3.79 5800
 C5H11O3r_39=C5H10O_olef_2+HO2 5.77E9 0.930 29799.3
 C4H71-3+CH3=CC(C)C*C 1.00E+13 0.00 0.00
 C4H71-3+OH=C4H8O_olef_1 1.00E+13 0.00 0.00
 C*C(C)CJCOH+HO2=C5H10O3_olef_2 8.39E9 0.600 -2105.6
 DUP
 IC4H7+C5H12O=IC4H8+C5H11Or_18.52E13 0.000 29516.5
 O2+C5H10O_olef_2=HO2+C5H9Or_olef_4 3.00E13 0.000 54105.7
 O2+C5H11O3r_10=C5H11O5r_16 2.02E13 -0.310 -337.0
 DUP
 C5H11O4r_5=CH3+C4H8O4 1.20E14 0.220 14098.6
 C5H11O3r_40=C5H11O3r_37 7.68E12 -0.130 34358.6
 PC2H4OH+Prenol=C2H5OH+C*C(C)CJCOH 1.25E12 0.000 15128.7
 Prenol+OH=C5H11O2r 7.80E7 1.290 -2652.9
 CH3+C5H12O=CH4+C5H11Or_1 2.38E13 0.000 17255.8
 CH3CHCHO+Prenol=C2H5CHO+CC(C)*CCJOH 2.17E13 0.000 20577.9
 CH2CHO+Prenol=CH3CHO+C*C(C)CJCOH 5.64E12 0.000 19048.3
 O2+C5H11O2r=C5H11O4r_18 2.46E11 0.400 -800.6
 DUP
 H+C5H10O_olef=H2+CC(C)*CCJOH 5.78E13 0.000 6190.1
 CC(C)CCJOH=C5H11Or_1 9.00E11 0.000 28966.8
 CH3O2+C5H12O=CH3O2H+CC(C)CJCOH 6.32E1 3.370 13718.6
 C5H11O3r_8=C5H10O2_8+OH 9.16E15 -1.080 18438.9
 C2H5O3r=C2H4O2+OH 9.00E14 0.000 1500.9
 C2H5+C5H12O=C2H6+C5H11Or_1 3.78E12 0.000 18546.4
 IC4H7-11+Isoprenol=IC4H8+C*C(C)CJCOH 7.46E12 0.000 9034.2
 C4H71-4+C5H12O=C4H8-1+CCJ(C)CCOH 1.67E12 0.000 14077.1
 O2+C5H11O3r_15=C5H11O5r_47 2.46E11 0.400 -800.6
 DUP
 C3H5-A+C5H10O_olef=C3H6+CC(C)*CCJOH 1.19E13 0.000 22967.9
 CH2CHO+C5H10O_olef=CH3CHO+C5H9Or_olef_12.12E13 0.000 22896.2
 CH3CHCHO+Isoprenol=C2H5CHO+C*C(C)CJCOH 2.17E13 0.000 20577.9
 IC4H9+C5H12O=IC4H10+CCJ(C)CCOH 6.83E11 0.000 13121.1
 C*CCJ(C)OH+CH3=C5H10O_olef_2 1.00E+13 0.00 0.00
 CH3CHCHO+Prenol=C2H5CHO+C*C(C)CJCOH 1.01E13 0.000 22250.9
 CH3+C5H12O=CH4+CC(C)CCJOH 1.70E13 0.000 13766.4
 C5H11O5r_16=C5H10O3+HO2 7.80E8 1.128 10630.7
 PC2H4OH+Isoprenol=C2H5OH+C*C(C)CJCOH 2.69E12 0.000 13455.7
 C5H9O2r_olef_4=C5H8O2_olef_3+H 1.76E10 1.000 18548.8
 O2+C5H9O3r_olef_13=C5H9O5r_olef_18 1.45E7 1.590 1080.3
 DUP
 IC4H9+C5H10O_olef=IC4H10+CC(C)*CCJOH 3.65E11 0.000 11041.8
 O2+C5H11O3r_9=C5H11O5r_6 7.54E14 -0.920 -129.1
 DUP

IC3H7+C5H12O=C3H8+CCJ(C)CCOH	2.14E12	0.000	14698.5
O2+C5H12O=HO2+C5H11Or_1	3.00E13	0.000	53567.7
C5H7O3r_olef_1=C5H6O3_olef+H1	7.76E10	1.000	18548.8
NC3H7+C5H12O=C3H8+CCJ(C)CCOH	1.11E12	0.000	13407.9
C5H11O4r_7=C5H10O3_6+OH	9.16E15	-1.080	18438.9
!C5H11O2r=SC4H7OH-I+CH2OH	7.68E13	0.000	30501.3
C5H11O2r=SC4H7OH-I+CH2OH	1.2E+12	0.46	27100
C5H9O3r_10=IC3H7+C2H2O3	6.00E13	0.220	14098.6
C5H11O3r_28=C5H10O2_1+OH	9.16E15	-1.080	18438.9
C3H5-A+CC(C)CC*O=C3H6+C5H9Or4	4.19E13	0.000	29516.5
C3H5-S+C5H10O_olef=C3H6+CC(C)*CCJOH	5.34E12	0.000	5903.3
C4H7O3r_1=CH3COCHO+CH2OH	9.00E13	0.220	14098.6
C5H9Or_olef_4=B13DE2M+OH	6.00E13	0.000	26799.1
C5H11O3r_10=C5H10O2_4+OH	3.50E10	0.100	9330.6
CH3O2+C5H12O=CH3O2H+CCJ(C)CCOH	6.50E2	3.010	12093.4
C3H5-T+C5H12O=C3H6+CCJ(C)CCOH	7.40E12	0.000	8986.4
IC4H9+Prenol=IC4H10+CC(C)*CCJOH	1.10E12	0.000	12499.7
IC3H7+C5H10O_olef=C3H8+CC(C)*CCJOH	1.14E12	0.000	12619.2
O2+C5H11O3r_25=C5H11O5r_37	7.54E14	-0.920	-129.1
DUP			
C4H7O2r_olef=IC3H5CHO+OH	2.70E15	0.000	1500.9
C3H5-A+Prenol=C3H6+C(C)CJCOH	1.66E13	0.000	26098.8
C3H3+C5H10O_olef_2=C3H4-A+C5H9Or_olef_4	4.52E13	0.000	26266.1
C5H9O3r_olef_4=C5H8O_olef_1+HO2	5.77E9	0.930	29799.3
C4H71-3+C5H12O=C4H8-2+CCJ(C)CCOH	9.78E12	0.000	25047.2
C5H11O3r_15=Prenol+HO2	3.66E10	0.790	15099.6
C5H9O3r_olef=IC4H7CHO+HO2	7.80E8	1.128	10630.7
C3H3+C5H10O_olef=C3H4-P+CC(C)*CCJOH	3.15E12	0.000	19287.3
C4H71-4+C5H12O=C4H8-1+C5H11Or_1	3.82E12	0.000	18546.4
C3H5-S+CC(C)CC*O=C3H6+CCJ(C)CC*O	1.31E13	0.000	8412.8
C5H11O5r_20=IIC4H7Q2-I+CH2O	9.00E13	0.220	14098.6
IC4H9+C5H10O_olef_2=IC4H10+C5H9Or_olef_4	2.02E12	0.000	18020.6
C5H9O2r_olef_1=IC4H7-I1+HOCHO	5.40E14	0.000	23890.4
O2+C5H11O3r_9=C5H11O5r_6	7.54E14	-0.920	-129.1
DUP			
CH2OH+C5H12O=CH3OH+CC(C)CCJOH	1.25E13	0.000	18259.6
C5H9Or=C*CCC*O+CH3	7.68E13	0.000	30615.9
C5H11O3r_15=C5H10O2_2+OH	4.56E8	1.290	9889.8
O2+C5H11O3r_2=C5H11O5r_3	1.30E11	0.230	-1579.8
DUP			
C5H9O3r=IC3H6CHO+HOCHO	9.00E13	0.220	14098.6
CH3+C5H12O=CH4+CCJ(C)CCOH	1.03E13	0.000	12786.5
C5H11O4r_18=C5H11O4r_21	1.64E11	0.130	19468.9
OH+C5H12O=H2O+CCJ(C)CCOH	1.72E13	0.000	2260.0
Prenol+CH3=C6H13Or_1	1.11E12	0.000	11065.7
DUP			
NC3H7+Prenol=C3H8+C(C)CJCOH	8.25E11	0.000	14459.5
HO2+CC(C)CC*O=H2O2+CC(C)CCJ(*O)	1.18E-4	4.900	3680.6
C5H11O5r_25=C5H10O4_7+OH	3.87E7	0.960	14289.8
O2+C5H11O3r_30=C5H11O5r_25	1.30E11	0.230	-1579.8
DUP			
C2H5+C5H12O=C2H6+CC(C)CJCOH	2.76E12	0.000	16252.0
CH3O2+Isoprenol=CH3O2H+C(C)CCJOH	2.46E-5	5.260	7480.7
C3H5-S+Prenol=C3H6+C(C)CJCOH	7.46E12	0.000	9034.2
O2+C5H9O3r_olef_10=C5H9O5r_olef_3	1.45E7	1.590	1080.3
DUP			
C5H10O4_14=C5H9O3r_13+OH	1.59E20	-1.500	42857.5
C4H71-3+Isoprenol=C4H8-2+C(C)CCJOH	2.10E13	0.000	26457.3

C5H9Or=C3H6+CH2CHO 3.72E13 0.000 22920.1
O2+C5H11Or_1=C5H11O3r_4 1.30E11 0.230 -1579.8
DUP
O2+C5H11O3r_25=C5H11O5r_37 7.54E14 -0.920 -129.1
DUP
Prenol+CH3=C6H13Or_1 1.11E12 0.000 11065.7
DUP
O2+C5H11O3r_8=C5H11O5r_2 1.30E11 0.230 -1579.8
DUP
O2+CC(C)CCJOH=C5H11O3r_26 2.02E13 -0.310 -337.0
DUP
C*C(COJ)CCOH=C4H7Or_olef+CH2O 2.70E14 0.000 23890.4
H+CC(C)CC*O=H2+CC(C)CCJ(*O) 7.15E5 2.400 1577.4
O2+C5H11O3r_6=C5H11O5r_9 7.54E14 -0.920 -129.1
DUP
C4H71-4+CC(C)CC*O=C4H8-1+C5H9Or_2 1.80E12 0.000 13670.8
IC3H7+Prenol=C3H8+C*C(C)CJCOH 1.60E12 0.000 15750.1
IC4H7-I1+CC(C)CC*O=IC4H8+C5H9Or_2 1.08E13 0.000 7576.3
C5H11O4r_21=C5H11O3_13+OH 4.58E15 -1.080 18438.9
C5H11O3r=Isoprenol+HO2 1.83E10 0.790 15099.6
C3H3+C5H10O_olef=C3H4-A+CC(C)*CCJOH 6.30E12 0.000 19287.3
PC2H4OH+Isoprenol=C2H5OH+C*C(CJ)CCOH 1.25E12 0.000 15128.7
IC4H7-I1+Isoprenol=IC4H8+C*C(C)CCJOH 2.16E13 0.000 9392.7
CH3O2+Prenol=CH3O2H+C*C(C)CJCOH 7.68E-2 4.400 13546.5
NC3H7+CC(C)CC*O=C3H8+C5H9Or_2 1.20E12 0.000 13001.6
O2+C5H11O3r_7=C5H11O5r_13 2.02E13 -0.310 -337.0
DUP
C4H71-3+CC(C)CC*O=C4H8-1+C5H9Or_2 1.43E13 0.000 26051.0
O2+C5H11O3r_23=C5H11O5r_39 2.02E13 -0.310 -337.0
DUP
C4H71-4+Prenol=C4H8-1+C*C(C)CJCOH 1.25E12 0.000 15128.7
C4H8O4=C4H7O3r_1+OH 1.59E20 -1.500 42857.5
C4H71-4+C5H10O_olef=C4H8-1+C5H9Or_olef_1 5.02E12 0.000 18976.6
H+IC4H7CHO=H2+C*C(C)CCJ(*O) 7.15E5 2.400 1577.4
HO2+C5H12O=H2O2+CCJ(C)CCOH 6.50E2 3.010 12093.4
CH3+CC(C)CC*O=CH4+C5H9Or_2 1.11E13 0.000 12380.2
C4H71-3+CC(C)CC*O=C4H8-2+C5H9Or 2.04E13 0.000 29516.5
C5H10O_olef+HOCHO=CC(C)CC*O+HOCHO 1.87E-2 3.286 -4509.9
DUP
C3H3+C5H10O_olef_2=C3H4-P+C5H9Or_olef_4 1.53E13 0.000 26266.1
C5H10O3_olef_1=C5H9O2r_olef_7+OH 1.59E20 -1.500 42857.5
C3H5-T+CC(C)CC*O=C3H6+C5H9Or_1 1.71E13 0.000 13455.7
C3H3+C5H12O=C3H4-P+CC(C)CJCOH 8.91E12 0.000 23541.5
O2+C5H11O3r_25=C5H11O5r_37 7.54E14 -0.920 -129.1
DUP
C3H3+C5H12O=C3H4-A+CC(C)CCJOH 1.82E13 0.000 22346.5
C3H5-A+CC(C)CC*O=C3H6+C5H9Or_2 2.32E13 0.000 24640.9
C5H11O3r_40=C5H10O_olef_2+HO2 8.66E9 0.930 29799.3
O2+C5H9O3r_olef_13=C5H9O5r_olef_9 1.45E7 1.590 1080.3
DUP
C3H5-T+C5H10O_olef=C3H6+CC(C)*CCJOH 3.96E12 0.000 6907.1
C2H3+C5H10O_olef=C2H4+C5H9Or_olef_1 3.01E13 0.000 12882.1
C4H71-3+C5H12O=C4H8-1+C5H11Or_1 2.55E13 0.000 30926.6
C4H71-4+C5H12O=C4H8-1+CC(C)CJCOH 2.76E12 0.000 16252.0
PC2H4OH+C5H10O_olef_2=C2H5OH+C5H9Or_olef_4 5.01E12 0.000 18976.6
CH2OH+C5H12O=CH3OH+C5H11Or_11 1.63E13 0.000 21749.0
HO2+C5H12O=H2O2+CC(C)CJCOH 6.32E1 3.370 13718.6
O2+C5H11O3r_23=C5H11O5r_39 2.02E13 -0.310 -337.0

DUP

C3H3+CC(C)CC*O=C3H4-P+C5H9Or_2 6.37E12 0.000 20960.3
C5H7O3r_olef_4=C4H5O2r_olef+CH2O 8.10E14 0.000 23890.4
C4H71-3+C5H12O=C4H8-2+CC(C)CCJOH 1.60E13 0.000 26027.1
C5H11O4r_5=CH3COCH3+C2H5O3r 6.00E13 0.220 14098.6
C3H5-T+Isoprenol=C3H6+C*(C)CCJOH 1.60E13 0.000 10396.5
O2+Prenol=HO2+C*(C)CJCOH 3.00E13 0.000 38804.3
C5H9Or_olef_4=C4H6O_olef_5+CH3 7.74E13 0.000 29922.8
H+C5H12O=H2+CC(C)CJCOH 2.33E14 0.000 9942.4
C2H5+Prenol=C2H6+C*(C)CJCOH 1.25E12 0.000 15128.7
C5H11O4r_1=C5H10O2_olef+HO2 5.77E9 0.930 29799.3
C5H10O4_5=C5H9O3r_4+OH 1.59E20 -1.500 42857.5
C3H3+C5H12O=C3H4-A+CCJ(C)CCOH 1.11E13 0.000 21366.6
NC3H7+CC(C)CC*O=C3H8+CCJ(C)CC*O 1.45E12 0.000 13838.1
C5H11O4r_1=C5H11O4r_3 2.91E12 -0.230 22298.7
CH3O2+C5H12O=CH3O2H+CC(C)CCJOH 2.46E-5 5.260 7480.7
C5H11O3r_5=C5H11O3r_7 1.64E11 0.130 19468.9
IC3H7+C5H12O=C3H8+C5H11Or_1 4.63E12 0.000 19167.8
C5H11O3r_25=C5H10O2_18+OH 2.28E8 1.290 9889.8
O2+CC(C)*CCJOH=C5H9O3r_olef_7 1.45E7 1.590 1080.3

DUP

C3H5-T+CC(C)CC*O=C3H6+CCJ(C)CC*O 9.71E12 0.000 9416.6
PC2H4OH+C5H12O=C2H5OH+C5H11Or_1 3.86E12 0.000 18546.4
CH3O2+Prenol=CH3O2H+CC(C)*CCJOH 5.12E-2 4.400 13546.5
Ccy(C*COCC*O)+H=Ccy(CJCOCC*O) 2.60E+13 0.000 1560
Ccy(CJCOCC*O)+O2=HO2+Ccy(C*COCC*O) 1.58E+12 0.000 15200
C5H8O4_olef_4=C5H7O3r_olef_4+OH 1.59E20 -1.500 42857.5
C4H71-3+C5H10O_olef_2=C4H8-2+C5H9Or_olef_4 2.63E13 0.000 29946.7
O2+C5H9O3r_olef_13=C5H9O5r_olef_9 1.45E7 1.590 1080.3

DUP

OH+Isoprenol=H2O+C*(C)CCJOH 5.10E4 2.600 -3178.7
C4H71-4+Isoprenol=C4H8-1+C*(C)CJCOH 2.69E12 0.000 13455.7
OH+C5H12O=H2O+CC(C)CCJOH 5.10E4 2.600 -3178.7
CC(CJ)*CC(*O)=IC4H7+CO 4.85E+12 0.261 47443
Ccy(CJCOCC*O)=CC(CJ)*CC(*O) 1.05E+13 0.085 22555
C5H11O3r_4=Isoprenol+HO2 2.88E9 0.930 29799.3
O2+C5H11Or_1=C5H11O3r_4 1.30E11 0.230 -1579.8

DUP

O2+C5H12O=HO2+CC(C)CJCOH 2.00E13 0.000 49853.8
IC4H7-I1+C5H10O_olef=IC4H8+C5H9Or_olef_1 3.01E13 0.000 12882.1
Prenol+H=CCJ(C)CCOH 7.62E13 0.000 4206.4
CH3O2+CC(C)CC*O=CH3O2H+CCJ(C)CC*O 6.50E2 3.010 12093.4
C5H9O2r_2=CH3COCH3+CH2CHO 6.00E13 0.220 14098.6
H+C5H10O_olef=H2+C5H9Or_olef_1 3.36E14 0.000 12595.3
O2+C5H11O3r_30=C5H11O5r_25 1.30E11 0.230 -1579.8

DUP

C4H71-4+CC(C)CC*O=C4H8-1+C5H9Or 3.82E12 0.000 18546.4
C5H10O3_olef_2=C5H9O2r_olef_4+OH 1.59E20 -1.500 42857.5
OH+Isoprenol=H2O+C*(C)CJCOH 1.50E5 2.400 -932.1
IC4H7-I1+Prenol=IC4H8+CC(C)*CCJOH 1.61E13 0.000 7361.2
C5H11O3r=C5H10O2_13+OH 2.28E8 1.290 9889.8
C3H3+Isoprenol=C3H4-A+C*(C)CJCOH 2.85E13 0.000 20745.2
IC3H7+Prenol=C3H8+CC(C)*CCJOH 3.45E12 0.000 14077.1
NC3H7+C5H10O_olef=C3H8+C5H9Or_olef_1 3.31E12 0.000 18307.4
O2+C5H11O3r_10=C5H11O5r_16 2.02E13 -0.310 -337.0

DUP

C4H71-4+C5H12O=C4H8-1+CC(C)CCJOH 2.75E12 0.000 15057.0
NC3H7+C5H12O=C3H8+CC(C)CJCOH 1.83E12 0.000 15582.8

C2H3+Prenol=C2H4+CC(C)*CCJOH1.61E13 0.000 7361.2
O2+CC(C)*CCJOH=C5H9O3r_Olef_7 1.45E7 1.590 1080.3
DUP
C5H9O3r_15=CH3+C4H6O3_2 1.20E14 0.220 14098.6
IC4H7+CC(C)CC*O=IC4H8+C5H9Or_2 4.72E13 0.000 24640.9
IC3H7+CC(C)CC*O=C3H8+C5H9Or 4.63E12 0.000 19167.8
PC2H4OH+C5H10O_Olef=C2H5OH+C5H9Or_Olef_1 5.03E12 0.000 18976.6
C6H13Or_1=CC(C)*CC+CH2OH 7.84E13 0.000 26433.4
IC4H7-Il+Isoprenol=IC4H8+C*(C)CJCOH 1.61E13 0.000 7361.2
C5H11O4r_13=C3H6OOH2-2+C2H4O2 6.00E13 0.220 14098.6
CH2OH+C5H10O_Olef=CH3OH+CC(C)*CCJOH 4.05E12 0.000 15200.4
CC(C)*CCJOH+HO2=C5H10O3_Olef_6 8.39E9 0.600 -2105.6
DUP
C3H5-S+C5H12O=C3H6+CCJ(C)CCOH 9.99E12 0.000 7982.6
Prenol+H=CC(C)CJCOH 1.79E13 0.000 5616.5
C3H3+C5H12O=C3H4-P+CC(C)CCJOH 9.19E12 0.000 22346.5
C5H9O2r=C3H6CHO-2+CH2O 9.00E13 0.220 14098.6
CH3O2+Isoprenol=CH3O2H+C*(C)CJCOH 5.12E-2 4.400 13546.5
CH2OH+Isoprenol=CH3OH+C*(C)CJCOH 1.22E13 0.000 16658.3
IC4H9+CC(C)CC*O=IC4H10+C5H9Or 1.56E12 0.000 17590.4
C3H5-A+Isoprenol=C3H6+C*(C)CJCOH 1.66E13 0.000 26098.8
CH3+CC(C)CC*O=CH4+CC(C)CCJ(*O) 5.00E0 3.600 4328.3
IC4H7+Prenol=IC4H8+C*(C)CJCOH 3.32E13 0.000 26098.8
O2+C5H9O3r_Olef_10=C5H9O5r_Olef_7 1.45E7 1.590 1080.3
DUP
C3H5-S+C5H12O=C3H6+CC(C)CJCOH 1.65E13 0.000 10157.5
C5H11O3r_16=C5H11O3r_23 4.66E7 1.400 28658.5
IC4H9+Prenol=IC4H10+C*(C)CJCOH 5.10E11 0.000 14172.7
O2+C5H9O3r_Olef_13=C5H9O5r_Olef_9 1.45E7 1.590 1080.3
DUP
C2H3+CC(C)CC*O=C2H4+C5H9Or_21.08E13 0.000 7576.3
NC3H7+C5H10O_Olef=C3H8+CC(C)*CCJOH 5.91E11 0.000 11328.6
C4H71-4+CC(C)CC*O=C4H8-1+CCJ(C)CC*O 2.19E12 0.000 14507.3
C3H5-T+C5H10O_Olef=C3H6+C5H9Or_Olef_1 2.23E13 0.000 13885.9
C2H3+Isoprenol=C2H4+C*(C)CJCOH 7.46E12 0.000 9034.2
!O2+Isoprenol=HO2+C*(C)CJCOH 2.00E13 0.000 34535.3
IC4H7+CC(C)CC*O=IC4H8+C5H9Or 8.52E13 0.000 29516.5
C5H10O_Olef+HOCHO=CC(C)CC*O+HOCHO 1.87E-2 3.286 -4509.9
DUP
NC3H7+Isoprenol=C3H8+C*(C)CJCOH 1.78E12 0.000 12786.5
CC(C)CCJOH=IC3H7+C2H3OH 2.47E14 0.000 27437.2
C5H11O3r_7=C5H10O2_1+OH 4.58E15 -1.080 18438.9
C3H3+Prenol=C3H4-P+C*(C)CJCOH 4.40E12 0.000 22418.2
CH2OH+Prenol=CH3OH+CC(C)*CCJOH 1.22E13 0.000 16658.3
C5H11O3r_16=C5H10O_Olef+HO2 5.77E9 0.930 29799.3
OH+IC4H7CHO=H2O+C*(C)CCJ(*O) 6.13E4 2.700 -4588.8
C3H3+CC(C)CC*O=C3H4-P+C5H9Or 1.18E13 0.000 25835.9
HO2+CC(C)CC*O=H2O2+CCJ(C)CC*O 6.50E2 3.010 12093.4
C2H5+Prenol=C2H6+CC(C)*CCJOH 2.69E12 0.000 13455.7
C3H5-A+C5H10O_Olef_2=C3H6+C5H9Or_Olef_4 5.41E13 0.000 29946.7
CC(C)CJCOH=CH3+C4H8O_Olef_1 9.32E13 0.000 30424.7
CH2CHO+CC(C)CC*O=CH3CHO+C5H9Or 1.61E13 0.000 22466.0
IC3H7+C5H12O=C3H8+CC(C)CCJOH 3.53E12 0.000 15678.4
O2+CCJ(C)CCOH=C5H11O3r_5 2.46E11 0.400 -800.6
CH3CHCHO+C5H12O=C2H5CHO+C5H11Or_1 2.67E13 0.000 25668.6
O2+C5H11O3r_6=C5H11O5r_9 7.54E14 -0.920 -129.1
DUP
IC4H7+CC(C)CC*O=IC4H8+CCJ(C)CC*O 5.34E13 0.000 25477.4

C4H71-3+Prenol=C4H8-2+CC(C)*CCJOH 1.79E13 0.000 24425.8
C2H3+C5H12O=C2H4+CC(C)CCJOH 1.65E13 0.000 8962.5
C4H71-3+Isoprenol=C4H8-2+C*(CJ)CCOH 8.13E12 0.000 26098.8
CH3+C5H12O=CH4+CC(C)CJCOH 1.70E13 0.000 14961.4
O2+C5H1103r_23=C5H1105r_39 2.02E13 -0.310 -337.0
DUP
IC4H9+C5H12O=IC4H10+CC(C)CCJOH 1.13E12 0.000 14101.0
CC(C)CJCOH=CC(C)C*O+OH 3.00E13 0.000 26799.1
C5H1103r_36=C5H1002_25+OH 2.28E8 1.290 9889.8
IC4H9+CC(C)CC*O=IC4H10+CC(C)CC*O 8.96E11 0.000 13551.3
C3H5-A+C5H12O=C3H6+C5H11Or_14.19E13 0.000 29516.5
IC4H7CHO+H=C*(C)CCJOH 3.30E14 0.000 10700.0
CH2CHO+Isoprenol=CH3CHO+C*(C)CJCOH 1.22E13 0.000 17375.3
IC3H7+CC(C)CC*O=C3H8+C5H9Or_2 2.31E12 0.000 14292.2
C5H9O2r_olef_1=C5H8O2_olef+H1.17E10 1.000 18548.8
C*(C)CJCOH+HO2=C*(COOH)CCOH 3.36E10 0.600 -2105.6
PC2H4OH+Isoprenol=C2H5OH+C*(C)CCJOH 3.61E12 0.000 15487.2
C5H1103r_9=C5H1002_7+OH 4.58E15 -1.080 18438.9
C3H5-A+Prenol=C3H6+CC(C)*CCJOH 3.58E13 0.000 24425.8
CH2OH+Isoprenol=CH3OH+C*(C)CCJOH 1.64E13 0.000 18689.8
C4H71-4+Prenol=C4H8-1+CC(C)*CCJOH 2.69E12 0.000 13455.7
C3H3+C5H12O=C3H4-A+CC(C)CJCOH 1.76E13 0.000 23541.5
C2H3+C5H12O=C2H4+C5H11Or_1 2.31E13 0.000 12451.9
O2+C5H1102r=C5H1104r_18 2.46E11 0.400 -800.6
DUP
C5H1102r_2=CH3+C4H8O2_olef_19.39E13 0.000 29731.6
C3H3+CC(C)CC*O=C3H4-A+CC(C)CC*O 1.46E13 0.000 21796.8
C3H5-A+Isoprenol=C3H6+C*(C)CJCOH 3.58E13 0.000 24425.8
CH2OH+C5H12O=CH3OH+CC(C)CJCOH 1.23E13 0.000 19454.6
O2+C5H1103r_21=C5H1105r_42 1.30E11 0.230 -1579.8
DUP
CH3+IC4H7CHO=CH4+C*(C)CCJ(*O) 5.00E0 3.600 4328.3
C4H71-3+C5H10_olef=C4H8-1+CC(C)*CCJOH 7.66E12 0.000 24378.0
C3H3+Isoprenol=C3H4-P+C*(CJ)CCOH 4.40E12 0.000 22418.2
CH3O2+C5H12O=CH3O2H+C5H11Or_1 2.04E1 3.590 17160.2
H+CC(C)CC*O=H2+C5H9Or 3.36E14 0.000 12595.3
C3H3+C5H12O=C3H4-P+C5H11Or_11.18E13 0.000 25835.9
IC4H7-I1+C5H12O=IC4H8+CC(C)CCJOH 1.65E13 0.000 8962.5
PC2H4OH+C5H12O=C2H5OH+CC(C)CJCOH 2.76E12 0.000 16252.0
IC4H7+Isoprenol=IC4H8+C*(CJ)CCOH 3.32E13 0.000 26098.8
C5H1103r_5=Prenol+HO2 5.77E9 0.930 29799.3
C4H6O_olef_5+H=C*CCJ(C)OH 5.61E+13 0.00 2294
C2H5+C5H12O=C2H6+CCJ(C)CCOH 1.67E12 0.000 14077.1
CH3CHCHO+Isoprenol=C2H5CHO+C*(C)CCJOH 2.73E13 0.000 22609.4
CH3O2+C5H10_olef_2=CH3O2H+C5H9Or_olef_4 2.04E1 3.590 17160.2
C4H71-3+CC(C)CC*O=C4H8-2+C5H9Or_2 1.15E13 0.000 24640.9
O2+CC(C)CC*O=HO2+CCJ(C)CC*O 1.00E13 0.000 46932.5
IC4H7-I1+C5H12O=IC4H8+CC(C)CCOH 9.99E12 0.000 7982.6
C5H9O3r_8=CH3COCH3+C2H3O2r 6.00E13 0.220 14098.6
O2+C5H9O3r_olef_13=C5H9O5r_olef_18 1.45E7 1.590 1080.3
DUP
C3H5-S+Isoprenol=C3H6+C*(C)CCOH 7.46E12 0.000 9034.2
IC4H7-I1+C5H10_olef_2=IC4H8+C5H9Or_olef_4 3.01E13 0.000 12882.1
C3H3+CC(C)CC*O=C3H4-A+C5H9Or_2 1.27E13 0.000 20960.3
HO2+IC4H7CHO=H2O2+C*(C)CCJ(*O) 1.18E-4 4.900 3680.6
O2+C5H9O3r_olef_13=C5H9O5r_olef_18 1.45E7 1.590 1080.3
DUP
IC4H9+C5H12O=IC4H10+CC(C)CJCOH 1.13E12 0.000 15296.0

C3H3+CC(C)CC*O=C3H4-A+C5H9Or3.49E13 0.000 25835.9
CC(C)*CCJOH+HO2=C5H10O3_olef_6 8.39E9 0.600 -2105.6
DUP
NC3H7+C5H12O=C3H8+CC(C)CCJOH1.82E12 0.000 14387.8
O2+C5H9O3r_olef_10=C5H9O5r_olef_3 1.45E7 1.590 1080.3
DUP
C4H9O3r=IC3H6OHCHO+OH 1.80E15 0.000 1500.9
HO2+C5H10O_olef_2=H2O2+C5H9Or_olef_4 2.04E1 3.590 17160.2
C3H5-T+C5H12O=C3H6+CC(C)CJCOH 1.22E13 0.000 11161.3
C3H3+Isoprenol=C3H4-A+C*(C)CCJOH 3.57E13 0.000 22776.7
OH+Prenol=H2O+C*(C)CJCOH 1.56E6 2.300 -1362.3
IC4H7-I1+Prenol=IC4H8+C*(C)CJCOH 7.46E12 0.000 9034.2
C4H71-3+C5H10O_olef=C4H8-2+CC(C)*CCJOH 5.93E12 0.000 22967.9
IC3H7+C5H10O_olef=C3H8+C5H9Or_olef_1 6.10E12 0.000 19598.0
O2+C5H11O3r_21=C5H11O5r_42 1.30E11 0.230 -1579.8
DUP
C5H10O4_8=C5H9O3r_8+OH 1.59E20 -1.500 42857.5
C4H7O2r=CH3+CH3COCHO 1.20E14 0.220 14098.6
C2H5O2r=CH3CHO+OH 2.70E15 0.000 1500.9
C4H9O2r=IC3H7CHO+OH 1.80E15 0.000 1500.9
C2H5+C5H10O_olef=C2H6+CC(C)*CCJOH 8.92E11 0.000 11997.8
HO2+Isoprenol=H2O2+C*(C)CCOJH 7.68E-2 4.400 13546.5
O2+C5H11O3r_21=C5H11O5r_42 1.30E11 0.230 -1579.8
DUP
IC4H9+Isoprenol=IC4H10+C*(C)CJCOH 1.10E12 0.000 12499.7
HO2+Prenol=H2O2+C*(C)CJCOH 1.54E-1 4.400 13546.5
C3H3+Prenol=C3H4-A+C*(C)CJCOH 1.32E13 0.000 22418.2
HO2+Isoprenol=H2O2+C*(C)CJCOH 5.12E-2 4.400 13546.5
C5H11O3r_5=C5H11O3r_6 4.66E7 1.400 28658.5
C3H3+CC(C)CC*O=C3H4-P+CCJ(C)CC*O 7.37E12 0.000 21796.8
C2H3+Prenol=C2H4+C*(C)CJCOH7.46E12 0.000 9034.2
C3H3+Prenol=C3H4-P+CC(C)*CCJOH 9.49E12 0.000 20745.2
HO2+Isoprenol=H2O2+C*(C)CCJOH 2.46E-5 5.260 7480.7
CH3CHCHO+C5H12O=C2H5CHO+CC(C)CJCOH 2.01E13 0.000 23374.2
C4H71-3+Isoprenol=C4H8-1+C*(C)CJCOH 2.31E13 0.000 25835.9
CH3CHCHO+CC(C)CC*O=C2H5CHO+CCJ(C)CC*O 1.67E13 0.000 21629.5
CH2OH+C5H12O=CH3OH+CCJ(C)CCOJH 7.58E12 0.000 17279.7
IC4H7+C5H12O=IC4H8+CCJ(C)CCOJH 4.07E13 0.000 25047.2
O2+C5H11O3r_23=C5H11O5r_39 2.02E13 -0.310 -337.0
DUP
C4H71-3+C5H12O=C4H8-1+CC(C)CCJOH 2.00E13 0.000 27437.2
O2+C5H11O3r_21=C5H11O5r_42 1.30E11 0.230 -1579.8
DUP
PC2H4OH+CC(C)CC*O=C2H5OH+CCJ(C)CC*O 2.19E12 0.000 14507.3
CH3CHCHO+C5H12O=C2H5CHO+CCJ(C)CCOJH 1.27E13 0.000 21199.3
CH3CHCHO+CC(C)CC*O=C2H5CHO+C5H9Or 2.67E13 0.000 25668.6
CH3O2+C5H10O_olef=CH3O2H+CC(C)*CCJOH 2.56E-2 4.400 13546.5
CH3CHCHO+C5H12O=C2H5CHO+CC(C)CCJOH 2.08E13 0.000 22179.2
O2+CC(C)CC*O=HO2+C5H9Or_2 2.00E13 0.000 41950.9
OH+Isoprenol=H2O+C*(C)CJCOH7.80E5 2.300 -1362.3
C3H5-S+C5H12O=C3H6+CC(C)CCJOH 1.65E13 0.000 8962.5
HO2+CC(C)CC*O=H2O2+C5H9Or 2.04E1 3.590 17160.2
OH+C5H12O=H2O+C5H11Or_1 1.67E6 2.078 375.3
O2+C5H9O3r_olef_10=C5H9O5r_olef_7 1.45E7 1.590 1080.3
DUP
C3H5-T+C5H12O=C3H6+C5H11Or_11.71E13 0.000 13455.7
CH3CHCHO+C5H10O_olef=C2H5CHO+C5H9Or_olef_1 3.51E13 0.000 26098.8
C2H5+CC(C)CC*O=C2H6+CCJ(C)CC*O 2.19E12 0.000 14507.3

C4H71-4+Isoprenol=C4H8-1+C*(C)CCJOH	3.61E12	0.000	15487.2
Prenol+CH3=CC(C)(C)CJCOH	5.59E11	0.000	12428.0
C3H5-T+C5H8_Olef=C3H6+C5H7r_Olef_1	1.19E13	0.000	8365.0
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_63	2.90E7	1.590	1080.3
DUP			
C6H11r_Olef_4=C2H3+IC4H8	5.92E13	0.000	33005.9
C6H11r_Olef_11=C2H3+C4H8-2	2.54E13	0.000	32958.1
C5H9Or_Olef_41=C5H9Or_Olef_40	4.80E12	0.000	56523.5
O2+C5H10_Olef_1=HO2+C5H9r_Olef_3	3.00E13	0.000	50697.3
C*CC*CC+CH3=C6H11r_Olef_10	2.07E12	0.000	8747.4
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_63	2.90E7	1.590	1080.3
DUP			
C5H9O3r_Olef_86=C5H9O3r_Olef_87	2.91E12	-0.230	22298.7
O2+C5H9Or_Olef_20=C5H9O3r_Olef_71	2.90E7	1.590	1080.3
DUP			
C*CCC*C+H=C*CCCCJ	1.29E14	0.000	5377.5
AC5H9O-C=C5H8O_Olef_8+H	1.17E10	1.000	18548.8
C5H9Or_Olef_17=C2H4+C3H5Or_Olef	1.51E13	0.000	20745.2
O2+C5H9Or_Olef_33=C5H9O3r_Olef_115	2.90E7	1.590	1080.3
DUP			
O2+C5H9Or_Olef_10=C5H9O3r_Olef_47	2.90E7	1.590	1080.3
DUP			
C5H9O3r_Olef_38=C*CCC*O+CH2O2H	5.36E12	-0.080	10790.8
C3H5O2r_Olef=C2H3CHO+OH	1.00E12	0.000	0.0
B1E3M3J+HO2=C5H10O2_Olef_8	3.35E10	0.600	-2105.6
O2+C5H9Or_Olef_15=C5H9O3r_Olef_24	2.90E7	1.590	1080.3
DUP			
C5H9Or_Olef_24=C4H71-1+CH2O	8.10E14	0.000	23890.4
O2+C5H9Or_Olef_34=C5H9O3r_Olef_103	2.90E7	1.590	1080.3
DUP			
C5H9Or_Olef_29=C3H5-S+CH3CHO	5.40E14	0.000	23890.4
C5H9O3r_Olef_17=C2H3CHO+C2H5O2r	1.61E13	-0.080	10790.8
B1E3M3J+Prenol=CC(C)C*C+C*(C)CJCOH	8.48E11	0.000	27724.0
AC5H9-D+Prenol=AC5H10+CC(C)*CCJOH	2.69E12	0.000	13455.7
C3H5-A+C*CCC*C=C3H6+C*CC*CCJ3	3.85E13	0.000	22179.2
C2H3+C5H8_Olef=C2H4+C5H7r_Olef	3.01E13	0.000	12882.1
C5H9O3r_Olef_51=CH3CHCHCHO+CH2O2H	1.61E13	-0.080	10790.8
C5H7Or_Olef=C5H6O_Olef+H	5.87E9	1.000	18548.8
C*CCJCC+HO2=C5H10O2_Olef_3m	3.35E10	0.600	-2105.6
DUP			
AC5H9-C+HO2=C5H10O2_Olef_14	3.35E10	0.600	-2105.6
DUP			
C5H9Or_Olef_1m=C5H9Or_Olef_41	9.00E11	0.000	22824.5
C5H9O3r_Olef_56=C5H9O3r_Olef_51	2.91E12	-0.230	22298.7
C*CC*CC+OH=C5H9Or_Olef_10	7.80E7	1.290	-2652.9
DUP			
C5H9Or_Olef_10=C4H6O_Olef_4+CH3	2.56E14	0.000	38431.2
O2+C5H9Or_Olef_20=C5H9O3r_Olef_71	2.90E7	1.590	1080.3
DUP			
C2H3+B13DE2M=C2H4+B13DE2MJ	7.46E12	0.000	9034.2
C5H9O3r_Olef_45=C5H9O3r_Olef_40	2.91E12	-0.230	22298.7
C5H9Or_Olef_34=C5H9Or_Olef_35	7.20E12	0.000	51600.1
C5H9O3r_Olef_37=C5H9O3r_Olef_38	2.91E12	-0.230	22298.7
C3H5-A+C5H8_Olef=C3H6+C5H7r_Olef_1	3.58E13	0.000	24425.8
C3H5-T+B13DE2M=C3H6+B13DE2MJ	5.53E12	0.000	10038.0
C*CC*CC+CH3=C6H11r_Olef_9	1.20E12	0.000	11782.7
DUP			
CC5H9-A+Prenol=CC(C)C*C+C*(C)CJCOH	1.25E12	0.000	15128.7

C5H9Or_olef_29=C5H8O_olef_4+H 1.17E10 1.000 18548.8
C5H10O2_2+HO2=CC(C)(OH)CCHO+HO2 1.490E+005 1.670 6810.0
C5H7r_olef_1+Prenol=C*CC*CC+CC(C)*CCJOH 5.96E12 0.000 15176.5
O2+C5H9Or_olef_19=C5H9O3r_olef_75 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_20=C5H9O3r_olef_67 2.90E7 1.590 1080.3
DUP
AC5H9-A2=C2H5+C3H4-A 3.11E15 0.000 56595.2
C3H3+C5H8_olef=C3H4-P+C5H7r_olef 1.56E13 0.000 26266.1
C5H9O3r_olef_84=C4H7O2r_olef_1+CH2O 1.61E13 -0.080 10790.8
C5H10O2_olef_4m4=C5H9Or_olef_29+OH 1.59E20 -1.500 42857.5
C3H5-A+C*CC*CC=C3H6+C*CC*CCJ 1.66E13 0.000 26098.8
C5H9O3r_olef_128=IC3H5CHO+CH2O2H 1.61E13 -0.080 10790.8
B13DE2M+CH3=C6H11r_olef_2 1.20E12 0.000 11782.7
DUP
O2+C*CCCC=HO2+C*CCCCJ 3.00E13 0.000 52959.1
C6H11r_olef_9=C3H5-S+C3H6 4.19E13 0.000 33149.3
O2+C5H9Or_olef_34=C5H9O3r_olef_103 2.90E7 1.590 1080.3
DUP
C5H9Or_olef_26=C2H3CHO+C2H5 9.00E13 0.220 14098.6
C5H9Or_olef_41=C3H4-A+SC2H4OH 4.33E15 0.000 58674.5
C*CC*CCJ+HO2=C5H8O2_olef(m0) 6.70E10 0.600 -2105.6
DUP
C5H10O2_olef_10=C5H9Or_olef_44+OH 1.59E20 -1.500 42857.5
O2+C5H9Or_olef_20=C5H9O3r_olef_71 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_2m=C5H9O3r_olef_93 2.90E7 1.590 1080.3
DUP
C5H9O3r_olef_13m=C5H9O3r_olef_17 2.91E12 -0.230 22298.7
AC5H9-C+HO2=C5H10O2_olef_12 3.35E10 0.600 -2105.6
DUP
C5H9O3r_olef_89=C5H9O3r_olef_90 2.91E12 -0.230 22298.7
C5H10O2_olef_14=B2E2M1OJ+OH 1.59E20 -1.500 42857.5
C3H3+C*CCC*C=C3H4-A+C*CC*CCJ 1.02E13 0.000 18498.6
C*CCCCJ+Prenol=C*CCCC+C*(C)CJCOH 8.25E11 0.000 14459.5
O2+C5H9Or_olef_15=C5H9O3r_olef_24 2.90E7 1.590 1080.3
DUP
C5H9O3r_olef_60=C5H9O3r_olef_84 2.91E12 -0.230 22298.7
AC5H9-A2+Prenol=AC5H10+C*(C)CJCOH 3.32E13 0.000 26098.8
AC5H9O-C=C3H5-T+CH3CHO 5.40E14 0.000 23890.4
C*CCC*C+CH3=C6H11r_olef_13 3.67E12 0.000 9966.3
C5H10O2_olef_3m=C5H9Or_olef_24+OH 1.59E20 -1.500 42857.5
B1E3M3J=AC5H9-C 4.50E11 0.000 33794.6
C5H7r_olef+Prenol=C5H8_olef+CC(C)*CCJOH 2.69E12 0.000 13455.7
C5H9Or_olef_1m=C3H5-T+C2H3OH 8.35E13 0.000 33173.2
CH3+C5H8_olef=CH4+C5H7r_olef 3.10E13 0.000 17686.0
C5H7Or_olef_1=C4H5-N+CH2O 2.70E14 0.000 23890.4
AC5H9-C+HO2=C5H10O2_olef_12 3.35E10 0.600 -2105.6
DUP
C*CC*CC+OH=C5H9Or_olef_9 7.80E7 1.290 -2652.9
DUP
H+C*CC*CC=H2+C*CC*CCJ 7.28E13 0.000 9177.6
C2H5+B13DE2M=C2H6+B13DE2MJ 1.25E12 0.000 15128.7
C*CCJCC+Prenol=C*CCCC+C*(C)CJCOH 6.74E12 0.000 26839.7
O2+C5H9Or_olef_16=C5H9O3r_olef_32 2.90E7 1.590 1080.3
DUP
CH3+C*CCC*C=CH4+C*CC*CCJ 1.78E13 0.000 9918.5
C*CC*CC+CH3=C6H11r_olef_11 1.18E12 0.000 11448.1

DUP
C5H7r_Olef_1+Prenol=C5H8_Olef+C*C(C)CJCOH 1.02E13 0.000 27508.9
C3H3+C5H8_Olef=C3H4-A+C5H7r_Olef_1 2.85E13 0.000 20745.2
C5H9Or_Olef_19=C5H9Or_Olef_23 4.80E12 0.000 51289.4
AC5H9-D=AC5H9-A2 9.00E11 0.000 22824.5
CC5H9-A=C4H6+CH3 4.26E13 0.000 27317.7
C5H9Or_Olef_38=C2H4+CH2CCH2OH 7.81E13 0.000 34200.9
O2+C5H9Or_Olef_2m=C5H9O3r_Olef_95 2.90E7 1.590 1080.3
DUP
C5H9r_Olef_2+HO2=C5H10O2_Olef_4m4 6.70E10 0.600 -2105.6
DUP
C5H7r_Olef_1+Prenol=C5H8_Olef+CC(C)*CCJOH 2.31E13 0.000 25835.9
O2+C*CC*CC=HO2+C*CC*CCJ 3.00E13 0.000 31423.8
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_60 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_37=C2H4+PC3H4OH-2 7.81E13 0.000 34200.9
C*CC*CC+CH3=C6H11r_Olef_9 1.20E12 0.000 11782.7
DUP
C5H9O3r_Olef_117=C4H7O2r_Olef_3+CH2O 1.61E13 -0.080 10790.8
O2+C5H9Or_Olef_4=C5H9O3r_Olef_89 5.20E11 0.230 -1579.8
DUP
O2+C5H9Or_Olef_9=C5H9O3r_Olef_56 5.20E11 0.230 -1579.8
DUP
O2+CC(C)*CC=HO2+B1E3M3J 3.00E13 0.000 37093.4
O2+C5H9Or_Olef_34=C5H9O3r_Olef_99 2.90E7 1.590 1080.3
DUP
AC5H9-C+Prenol=CC(C)*CC+CC(C)*CCJOH 1.79E13 0.000 24425.8
C5H9r_Olef_3=C2H4+C3H5-S 6.93E13 0.000 36543.1
C*CC*CC+OH=C5H9Or_Olef_9 7.80E7 1.290 -2652.9
DUP
B13DE2M+H=CC5H9-A 5.06E13 0.000 6739.8
DUP
C5H10O2_Olef_12=AC5H9O-C+OH 1.59E20 -1.500 42857.5
C5H9O3r_Olef_87=C4H7O2r_Olef_2+CH2O 5.36E12 -0.080 10790.8
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_60 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_35=C5H9Or_Olef_38 9.00E11 0.000 39052.6
CH3+C*CC*CC=CH4+C*CC*CCJ 7.68E12 0.000 13838.1
C5H9Or_Olef_15=C5H9Or_Olef_16 9.00E11 0.000 35204.7
O2+C5H9Or_Olef_40=C5H9O3r_Olef_123 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_26=C2H3+C2H5CHO 8.10E14 0.000 23890.4
O2+C5H9Or_Olef_35=C5H9O3r_Olef_106 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_9=C5H9O3r_Olef_56 5.20E11 0.230 -1579.8
DUP
C3H5-S+C*CC*CC=C3H6+C*CC*CCJ 7.46E12 0.000 9034.2
B13DE2M+OH=C5H9Or_Olef_1m 7.80E7 1.290 -2652.9
DUP
AC5H9-C+Prenol=AC5H10+C*C(C)CJCOH 1.03E13 0.000 27508.9
C*CCCCJ+Prenol=C*CCCC+CC(C)*CCJOH 1.78E12 0.000 12786.5
O2+C5H9Or_Olef_32=C5H9O3r_Olef_86 3.02E15 -0.920 -129.1
DUP
O2+C5H9Or_Olef_34=C5H9O3r_Olef_99 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_16=C5H9O3r_Olef_35 2.90E7 1.590 1080.3
DUP
C5H9O3r_Olef_129=C5H9O3r_Olef_128 2.91E12 -0.230 22298.7

C5H9Or_Olef_40=C5H9Or_Olef_42 4.50E11 0.000 33794.6
O2+C5H9Or_Olef_33=C5H9O3r_Olef_112 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_22=C5H9O3r_Olef_73 5.20E11 0.230 -1579.8
DUP
C5H7r_Olef+Prenol=C5H8_Olef+C*(C)CJCOH 1.25E12 0.000 15128.7
C5H9O3r_Olef_40=C3H5O2r_Olef+CH3CHO 1.61E13 -0.080 10790.8
C*CC*CC+OH=C5H9Or_Olef_13 7.80E7 1.290 -2652.9
DUP
C3H3+B13DE2M=C3H4-A+B13DE2MJ 4.40E12 0.000 22418.2
C5H9Or_Olef_9=C3H5-S+C2H3OH 7.41E13 0.000 35515.4
C*CC*CCJ+Prenol=C*CCC*C+CC(C)*CCJOH 7.13E13 0.000 33555.6
O2+C5H9Or_Olef_15=C5H9O3r_Olef_29 2.90E7 1.590 1080.3
DUP
CH3+C5H8_Olef=CH4+C5H7r_Olef_1 1.66E13 0.000 12165.1
O2+C5H9Or_Olef_14=C5H9O3r_Olef_37 5.20E11 0.230 -1579.8
DUP
C3H3+C*CCC*C=C3H4-P+C*CC*CCJ 1.02E13 0.000 18498.6
C5H9r_Olef_3+Prenol=C5H10_Olef_1+CC(C)*CCJOH 2.69E12 0.000 13455.7
AC5H9O-C=IC3H5CHO+CH3 6.00E13 0.220 14098.6
C5H9r_Olef_2+HO2=C5H10O2_Olef_4m4 6.70E10 0.600 -2105.6
DUP
C*CCJCC+Prenol=C5H10_Olef_1+CC(C)*CCJOH 1.79E13 0.000 24425.8
C5H9Or_Olef_16=C5H9Or_Olef_17 7.20E12 0.000 54778.8
C5H9Or_Olef_34=C5H9Or_Olef_33 7.20E12 0.000 37929.3
C5H9Or_Olef_34=C4H6O_Olef_6+CH3 1.08E15 0.000 58674.5
O2+C5H9Or_Olef_34=C5H9O3r_Olef_103 2.90E7 1.590 1080.3
DUP
C*CC*CC+CH3=C6H11r_Olef_11 1.18E12 0.000 11448.1
DUP
B2E3M1OJ=IC4H7-I1+CH2O 5.40E14 0.000 23890.4
C3H5-S+C*CCC*C=C3H6+C*CC*CCJ 1.73E13 0.000 5114.6
CH3+B13DE2M=CH4+B13DE2MJ 7.68E12 0.000 13838.1
B2E2M1OJ=C4H72-2+CH2O 5.40E14 0.000 23890.4
B2E3M1OJ=CC(C)*CC*O+H 2.35E10 1.000 18548.8
O2+C5H9Or_Olef_10=C5H9O3r_Olef_47 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_26=C5H8O_Olef_2+H 1.76E10 1.000 18548.8
C3H3+C*CC*CC=C3H4-P+C*CC*CCJ 4.40E12 0.000 22418.2
C5H9Or_Olef_44=C5H8O_Olef_5+H 3.52E10 1.000 18548.8
AC5H9-D=C2H4+C3H5-T 7.81E13 0.000 34200.9
O2+C5H9Or_Olef_20=C5H9O3r_Olef_67 2.90E7 1.590 1080.3
DUP
C5H9r_Olef_2+Prenol=C5H10_Olef_1+CC(C)*CCJOH 4.62E13 0.000 25835.9
C2H5+C*CCC*C=C2H6+C*CC*CCJ 2.89E12 0.000 11209.1
C*CCCCJ=C3H5-A+C2H4 1.51E13 0.000 20745.2
AC5H9-C+HO2=C5H10O2_Olef_14 3.35E10 0.600 -2105.6
DUP
O2+C5H9Or_Olef_10=C5H9O3r_Olef_47 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_33=C4H612+CH2OH 7.35E15 0.000 67421.9
AC5H9-C+Prenol=AC5H10+CC(C)*CCJOH 2.31E13 0.000 25835.9
C5H10O2_Olef_1m=C5H9Or_Olef_26+OH 1.59E20 -1.500 42857.5
CC5H9-A=CC5H9-A 3.60E12 0.000 43067.8
C*CCC*C+H=C*CCCJC 1.11E14 0.000 3847.9
C2H5+C5H8_Olef=C2H6+C5H7r_Olef_1 2.69E12 0.000 13455.7
O2+C5H9Or_Olef_9=C5H9O3r_Olef_56 5.20E11 0.230 -1579.8
DUP

B13DE2M+H=AC5H9-C 5.03E13 0.000 2748.5
 C6H11r_olef_15=C3H5-A+C3H6 1.65E13 0.000 20649.6
 C5H9Or_olef_35=C5H9Or_olef_37 4.50E11 0.000 37642.5
 C*CCJCC+HO2=C5H10O2_olef_1m 3.35E10 0.600 -2105.6
 DUP
 C5H9r_olef_2+Prenol=C5H10_olef_1+C*(C)CJCOH 2.02E13 0.000 27508.9
 C5H9O3r_olef_90=C2H3COCH3+CH2O2H 1.61E13 -0.080 10790.8
 C*CC*CC+H=C5H9r_olef_2 5.03E13 0.000 2748.5
 H+B13DE2M=H2+B13DE2MJ 7.28E13 0.000 9177.6
 O2+C5H9Or_olef_10=C5H9O3r_olef_47 2.90E7 1.590 1080.3
 DUP
 O2+C5H9Or_olef_41=C5H9O3r_olef_119 1.16E8 1.590 1080.3
 DUP
 C*CC*CC+H=C*CCCJC 8.20E13 0.000 5377.5
 C3H5-S+B13DE2M=C3H6+B13DE2MJ 7.46E12 0.000 9034.2
 C6H11r_olef=C5H8_olef+CH3 7.35E15 0.000 67421.9
 C5H9Or_olef_10=C5H9Or_olef_15 1.50E11 0.000 40128.1
 C5H9Or_olef_24=C5H8O_olef(m14)+H 3.52E10 1.000 18548.8
 O2+C5H9Or_olef_1m=C5H9O3r_olef_129 5.20E11 0.230 -1579.8
 DUP
 O2+C*CCCC=HO2+C*CCCJC 2.00E13 0.000 48192.7
 O2+C5H9Or_olef_40=C5H9O3r_olef_121 2.90E7 1.590 1080.3
 DUP
 O2+C5H9Or_olef_34=C5H9O3r_olef_99 2.90E7 1.590 1080.3
 DUP
 C5H7Or_olef_3=C5H6O_olef_3+H 1.17E10 1.000 18548.8
 C5H7r_olef_1+Prenol=C*CC*CC+C*(C)CJCOH 2.76E12 0.000 16849.5
 B13DE2MJ+HO2=C*(C)C(C)C*CC 1.34E11 0.600 -2105.6
 C*CC*CC+CH3=C6H11r_olef_9 1.20E12 0.000 11782.7
 DUP
 AC5H9-A2+HO2=C5H10O2_olef_10 1.34E11 0.600 -2105.6
 O2+C5H9Or_olef_13=C5H9O3r_olef_13m 3.02E15 -0.920 -129.1
 DUP
 C*CCJCC+Prenol=C5H10_olef_1+C*(C)CJCOH 8.18E12 0.000 26098.8
 O2+C5H9Or_olef_10=C5H9O3r_olef_45 2.90E7 1.590 1080.3
 DUP
 C5H9Or_olef_32=C2H3+C3H5OH 4.20E13 0.000 36351.9
 O2+C5H9Or_olef_5m3=C5H9O3r_olef_63 2.90E7 1.590 1080.3
 DUP
 B13DE2M+CH3=C6H11r_olef_4 1.23E12 0.000 12882.1
 C*CCC*C+CH3=C6H11r_olef_15 1.80E12 0.000 11806.6
 DUP
 O2+C5H9Or_olef_42=C5H9O3r_olef_125 2.90E7 1.590 1080.3
 O2+C5H9Or_olef_16=C5H9O3r_olef_32 2.90E7 1.590 1080.3
 DUP
 O2+C5H9Or_olef_15=C5H9O3r_olef_29 2.90E7 1.590 1080.3
 DUP
 C3H3+B13DE2M=C3H4-P+B13DE2MJ 4.40E12 0.000 22418.2
 C4H7O2r_olef_3=C2H3COCH3+OH 3.00E12 0.000 0.0
 B1E3M3J+Prenol=CC(C)C*(C)C*CCJCOH 2.00E12 0.000 26051.0
 C5H9Or_olef_35=C2H5+C3H4O_olef 7.77E14 0.000 56595.2
 C6H11r_olef_13=C2H3+C4H8-1 4.20E13 0.000 36351.9
 O2+C*CCC*C=HO2+C*CC*CCJ 2.00E13 0.000 25825.9
 C5H10O2_olef_8=B1E3M3OJ+OH 1.59E20 -1.500 42857.5
 C*CC*CC+H=C5H9r_olef_3 7.85E13 0.000 5951.1
 DUP
 O2+C5H9Or_olef_13=C5H9O3r_olef_13m 3.02E15 -0.920 -129.1
 DUP

C5H9Or_olef_40=C4H6O_olef_7+CH3 1.08E15 0.000 58674.5
O2+C5H9Or_olef_20=C5H9O3r_olef_67 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_37=C5H9O3r_olef_111 5.20E11 0.230 -1579.8
DUP
C5H9Or_olef_10=C5H9Or_olef_14 7.20E12 0.000 55448.0
C5H9Or_olef_19=C4H6+CH2OH 3.72E14 0.000 35873.9
B2E2M1OJ=C5H8O_olef_7+H 2.35E10 1.000 18548.8
AC5H9-C+Prenol=CC(C)*CC+C*(C)CJCOH 8.23E12 0.000 26098.8
C5H7Or_olef=C2H3+C2H3CHO 5.40E14 0.000 23890.4
C*CC*CC+OH=C5H9Or_olef_9 7.80E7 1.290 -2652.9
DUP
O2+B13DE2M=HO2+B13DE2MJ 3.00E13 0.000 39297.3
C*CC*CCJ+HO2=C5H8O2_olef_2m 6.70E10 0.600 -2105.6
O2+C5H9Or_olef_15=C5H9O3r_olef_24 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_20=C5H9O3r_olef_71 2.90E7 1.590 1080.3
DUP
C5H8O2_olef(m0)=C5H7Or_olef_1+OH 1.59E20 -1.500 42857.5
O2+C5H9Or_olef_2m=C5H9O3r_olef_93 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_19=C5H9O3r_olef_78 2.90E7 1.590 1080.3
DUP
O2+CC(C)*CC=HO2+AC5H9-C 3.00E13 0.000 38758.2
C5H9O3r_olef_93=C5H9O3r_olef_117 2.91E12 -0.230 22298.7
C*(C)C(C)C=C5H7Or_olef_3+OH 1.59E20 -1.500 42857.5
O2+C5H9Or_olef_19=C5H9O3r_olef_75 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_1m=C5H9O3r_olef_129 5.20E11 0.230 -1579.8
DUP
C5H9Or_olef_2m=C5H9Or_olef_33 4.50E11 0.000 33794.6
HO2+B13DE2M=H2O2+B13DE2MJ 7.68E-2 4.400 13546.5
AC5H9-A2=AC5H9-C 9.60E12 0.000 48517.0
B1E3M3OJ=C2H3+CH3COCH3 5.40E14 0.000 23890.4
B1E3M3J+Prenol=CC(C)*CC+C*(C)CJCOH 8.05E12 0.000 26098.8
C5H9Or_olef_22=C2H4+C3H5Or_olef_1 1.51E13 0.000 20745.2
C*CCC*C+OH=C5H9Or_olef_14 1.56E8 1.290 -2652.9
DUP
C5H9Or_olef_29=CH3CHCHCHO+CH3 6.00E13 0.220 14098.6
C*CC*CC+H=C*CCJCC 6.11E13 0.000 3704.5
O2+C5H9Or_olef_38=C5H9O3r_olef_109 5.20E11 0.230 -1579.8
AC5H9-A2+Prenol=AC5H10+CC(C)*CCJOH 7.15E13 0.000 24425.8
AC5H9-D+Prenol=AC5H10+C*(C)CJCOH 1.25E12 0.000 15128.7
C3H5-T+C*CC*CC=C3H6+C*CC*CCJ5.53E12 0.000 10038.0
HO2+C*CC*CC=H2O2+C*CC*CCJ 7.68E-2 4.400 13546.5
C*CCJCC=C5H9r_olef_2 3.00E11 0.000 32121.6
C5H8O2_olef_2m=C5H7Or_olef+OH 1.59E20 -1.500 42857.5
C*CC*CC+CH3=C6H11r_olef_9 1.20E12 0.000 11782.7
DUP
CC5H9-A=C2H3+C3H6 4.19E13 0.000 33149.3
C*CC*CC+OH=C5H9Or_olef_5m3 7.80E7 1.290 -2652.9
C5H9Or_olef_44=C4H71-2+CH2O 8.10E14 0.000 23890.4
O2+C5H9Or_olef_20=C5H9O3r_olef_67 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_15=C5H9O3r_olef_29 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_olef_37=C5H9O3r_olef_111 5.20E11 0.230 -1579.8
DUP

B1E3M3J+HO2=C5H10O2_Olef_9 3.35E10 0.600 -2105.6
 O2+C5H9Or_Olef_40=C5H9O3r_Olef_121 2.90E7 1.590 1080.3
 DUP
 C5H9r_Olef_3+Prenol=C5H10_Olef_1+C*(C)CJCOH 1.25E12 0.000 15128.7
 O2+C5H9Or_Olef_13=C5H9O3r_Olef_13m 3.02E15 -0.920 -129.1
 DUP
 C5H9Or_Olef_13=C2H3+SC3H5OH 4.49E13 0.000 35324.2
 O2+C5H9Or_Olef_23=C5H9O3r_Olef_80 8.10E13 -0.310 -337.0
 DUP
 C*CCCJC=C2H3+C3H6 4.20E13 0.000 36351.9
 C2H3+C5H8_Olef=C2H4+C5H7r_Olef_1 1.61E13 0.000 7361.2
 B13DE2M+H=CC5H9-A 5.06E13 0.000 6739.8
 DUP
 C*(C)CJCOH=C*(C)CCOH 7.20E12 0.000 51600.1
 C3H3+C5H8_Olef=C3H4-P+C5H7r_Olef_1 9.49E12 0.000 20745.2
 C5H7Or_Olef_1=C5H6O_Olef_1+H1.17E10 1.000 18548.8
 O2+C5H9Or_Olef_9=C5H9O3r_Olef_56 5.20E11 0.230 -1579.8
 DUP
 B13DE2MJ+Prenol=B13DE2M+C*(C)CJCOH 3.32E13 0.000 26098.8
 C5H9Or_Olef_4=C5H9Or_Olef_4 3.60E12 0.000 43067.8
 O2+C5H9Or_Olef_33=C5H9O3r_Olef_115 2.90E7 1.590 1080.3
 DUP
 O2+C5H9Or_Olef_10=C5H9O3r_Olef_45 2.90E7 1.590 1080.3
 DUP
 C*CCJCC+HO2=C5H10O2_Olef_3m 3.35E10 0.600 -2105.6
 DUP
 O2+C5H9Or_Olef_32=C5H9O3r_Olef_86 3.02E15 -0.920 -129.1
 DUP
 C3H3+C*CC*CC=C3H4-A+C*CC*CCJ 4.40E12 0.000 22418.2
 C*CCJCC+HO2=C5H10O2_Olef_1m 3.35E10 0.600 -2105.6
 DUP
 O2+C5H10_Olef_1=HO2+C*CCJCC 3.00E13 0.000 37103.5
 C3H5-A+C5H8_Olef=C3H6+C5H7r_Olef 5.53E13 0.000 29946.7
 C*CCCJC+Prenol=C*CCCC+C*(C)CJCOH 1.60E12 0.000 15750.1
 C*CC*CC+OH=C5H9Or_Olef_9 7.80E7 1.290 -2652.9
 DUP
 O2+C5H9Or_Olef_10=C5H9O3r_Olef_45 2.90E7 1.590 1080.3
 DUP
 C6H11r_Olef_2=C3H6+C3H5-T 4.73E13 0.000 30807.1
 O2+C5H9Or_Olef_23=C5H9O3r_Olef_80 8.10E13 -0.310 -337.0
 DUP
 C*CC*CC+OH=C5H9Or_Olef_10 7.80E7 1.290 -2652.9
 DUP
 C4H7O2r_Olef_2=C*CCC*O+OH 1.00E12 0.000 0.0
 C5H9Or_Olef_20=C5H9Or_Olef_22 7.20E12 0.000 54778.8
 C*CC*CC+H=C5H9r_Olef_3 7.85E13 0.000 5951.1
 DUP
 C3H5-T+C*CCC*C=C3H6+C*CC*CCJ 1.28E13 0.000 6118.4
 C5H9Or_Olef_20=CH3+C4H6O_Olef_4 2.39E14 0.000 39458.9
 B13DE2MJ+Prenol=B13DE2M+CC(C)*CCJOH 7.15E13 0.000 24425.8
 B13DE2M+OH=C5H9Or_Olef_1m 7.80E7 1.290 -2652.9
 DUP
 O2+C*CCCC=HO2+C*CCJCC 2.00E13 0.000 35594.4
 B13DE2M+OH=C5H9Or_Olef_2m 7.80E7 1.290 -2652.9
 C*CC*CCJ+Prenol=C*CC*CC+CC(C)*CCJOH 3.58E13 0.000 24425.8
 O2+C5H9Or_Olef_14=C5H9O3r_Olef_37 5.20E11 0.230 -1579.8
 DUP
 O2+C5H9Or_Olef_4=C5H9O3r_Olef_89 5.20E11 0.230 -1579.8

DUP
C3H5-S+C5H8_Olef=C3H6+C5H7r_Olef 3.01E13 0.000 12882.1
B1E3M3J+Prenol=CC(C)*CC+CC(C)*CCJOH 1.79E13 0.000 24425.8
C2H3+C*CC*CC=C2H4+C*CC*CCJ 7.46E12 0.000 9034.2
C*CCJCC+Prenol=C*CCCC+CC(C)*CCJOH 1.53E13 0.000 25166.7
O2+C5H9Or_Olef_2m=C5H9O3r_Olef_95 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_15=C5H9O3r_Olef_24 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_23=C3H5-A+C2H3OH 5.92E13 0.000 21844.6
C5H9r_Olef_2+HO2=C5H10O2_Olef_4m4 6.70E10 0.600 -2105.6
DUP
O2+AC5H10=HO2+AC5H9-A2 3.00E13 0.000 39297.3
C*CC*CC+OH=C5H9Or_Olef_13 7.80E7 1.290 -2652.9
DUP
H+C5H8_Olef=H2+C5H7r_Olef 3.51E14 0.000 12786.5
C5H9Or_Olef_14=C3H5-A+C2H3OH 1.61E13 0.000 19717.5
C*CCCJC+Prenol=C*CCCC+CC(C)*CCJOH 3.45E12 0.000 14077.1
O2+C5H9Or_Olef_19=C5H9O3r_Olef_78 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_15=C5H9O3r_Olef_29 2.90E7 1.590 1080.3
DUP
B13DE2M+CH3=C6H11r_Olef_3 2.39E12 0.000 6787.6
C*CC*CCJ+Prenol=C*CC*CC+C*(C)CJCOH 1.49E13 0.000 26098.8
O2+C5H9Or_Olef_35=C5H9O3r_Olef_108 2.90E7 1.590 1080.3
DUP
C2H3+C*CCC*C=C2H4+C*CC*CCJ 1.73E13 0.000 5114.6
C5H9r_Olef_2+HO2=C5H10O2_Olef_4m4 6.70E10 0.600 -2105.6
DUP
C4H7O2r_Olef_1=CH3CHCHCHO+OH 3.00E12 0.000 0.0
O2+C5H9Or_Olef_33=C5H9O3r_Olef_112 2.90E7 1.590 1080.3
DUP
C*CCC*C+OH=C5H9Or_Olef_14 1.56E8 1.290 -2652.9
DUP
HO2+C*CCC*C=H2O2+C*CC*CCJ 5.12E-2 4.400 13546.5
B1E3M3OJ=C2H3COCH3+CH3 1.20E14 0.220 14098.6
C*CCCCJ=C*CCJCC 4.80E12 0.000 36877.7
O2+C5H9Or_Olef_13=C5H9O3r_Olef_13m 3.02E15 -0.920 -129.1
DUP
C5H7Or_Olef_3=C4H5-I+CH2O 2.70E14 0.000 23890.4
O2+C5H9Or_Olef_35=C5H9O3r_Olef_108 2.90E7 1.590 1080.3
DUP
C5H9Or_Olef_16=CH3+C4H6O_Olef_5 2.39E14 0.000 39458.9
C*CCJCC=C4H6+CH3 2.39E14 0.000 39458.9
C5H9Or_Olef_35=C5H9Or_Olef_33 4.80E12 0.000 36256.3
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_63 2.90E7 1.590 1080.3
DUP
O2+C5H10_Olef_1=HO2+C5H9r_Olef_2 2.00E13 0.000 33811.7
C*CC*CCJ+HO2=C5H8O2_Olef(m0) 6.70E10 0.600 -2105.6
DUP
C3H5-S+C5H8_Olef=C3H6+C5H7r_Olef_1 1.61E13 0.000 7361.2
C5H9Or_Olef_5m3=C5H9Or_Olef_20 6.00E11 0.000 33531.7
C3H5-T+C5H8_Olef=C3H6+C5H7r_Olef 2.23E13 0.000 13885.9
C3H5-A+B13DE2M=C3H6+B13DE2MJ 1.66E13 0.000 26098.8
C*CCC*C+OH=C5H9Or_Olef_32 1.56E8 1.290 -2652.9
C5H10O2_Olef_9=B2E3M1OJ+OH 1.59E20 -1.500 42857.5
C5H9Or_Olef_5m3=C5H9Or_Olef_19 9.00E11 0.000 35204.7
O2+C5H9Or_Olef_41=C5H9O3r_Olef_119 1.16E8 1.590 1080.3

DUP
O2+C5H9Or_Olef_17=C5H9O3r_Olef_36 5.20E11 0.230 -1579.8
B13DE2M+CH3=C6H11r_Olef_2 1.20E12 0.000 11782.7
DUP
O2+C5H9Or_Olef_42=C5H9O3r_Olef_124 2.90E7 1.590 1080.3
C*CC*CCJ+Prenol=C*CCC*C+C*(C)CJCOH 2.88E13 0.000 35228.6
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_60 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_16=C5H9O3r_Olef_35 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_34=C5H9O3r_Olef_103 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_40=C5H9O3r_Olef_123 2.90E7 1.590 1080.3
DUP
O2+C5H9Or_Olef_22=C5H9O3r_Olef_73 5.20E11 0.230 -1579.8
DUP
B13DE2M+H=AC5H9-D 1.57E14 0.000 5951.1
C5H7r_Olef=C2H4+C3H3 7.04E13 0.000 30711.5
B13DE2M+CH3=C6H11r_Olef 2.13E12 0.000 7241.7
O2+C5H9Or_Olef_5m3=C5H9O3r_Olef_60 2.90E7 1.590 1080.3
DUP
C*CC*CC+CH3=C6H11r_Olef_5 2.13E12 0.000 7241.7
C*CCC*C+CH3=C6H11r_Olef_15 1.80E12 0.000 11806.6
DUP
O2+C5H9Or_Olef_34=C5H9O3r_Olef_99 2.90E7 1.590 1080.3
DUP
C2H5+C*CC*CC=C2H6+C*CC*CCJ 1.25E12 0.000 15128.7
C5H9Or_Olef_2m=C5H9Or_Olef_34 3.00E11 0.000 32121.6
H+C*CCC*C=H2+C*CC*CCJ 2.01E14 0.000 6190.1
B13DE2M+H=B1E3M3J 5.61E13 0.000 2294.4
C2H5+C5H8_Olef=C2H6+C5H7r_Olef 4.98E12 0.000 18976.6
O2+C5H9Or_Olef_35=C5H9O3r_Olef_106 2.90E7 1.590 1080.3
DUP
C3H3+C5H8_Olef=C3H4-A+C5H7r_Olef 1.54E13 0.000 26266.1
O2+C5H9Or_Olef_10=C5H9O3r_Olef_45 2.90E7 1.590 1080.3
DUP
H+C5H8_Olef=H2+C5H7r_Olef_1 1.59E14 0.000 7361.2
CC5H9-A+Prenol=CC(C)C*C+CC(C)*CCJOH 2.69E12 0.000 13455.7
C*(C)C(OOH)C*O=C5H7O2r_Olef_4+OH 1.59E20 -1.500 42857.5
C5H7O2r_Olef_4=IC3H5CHO+HCO 9.00E13 0.220 14098.6
C3H5-A+CC(C)*CC*O=C3H6+CC(CJ)*CC(*O) 1.66E13 0.000 26098.8
C5H9O2r_2(m0)=CH3+C4H6O2_Olef_1 3.19E14 0.000 34822.3
C*(CJ)CC*O+HO2=C5H8O3_Olef_4 1.34E11 0.600 -2105.6
CC(CJ)*CC(*O)=C4H4O_Olef+CH3 1.08E15 0.000 58674.5
C5H9Or_2=C5H9Or 7.20E12 0.000 49234.0
C5H7O2r_Olef_4=C5H6O2_Olef_3+H 1.76E10 1.000 18548.8
CC(CJ)*CC(*O)+HO2=C5H8O3_Olef 3.35E10 0.600 -2105.6
DUP
CC(CJ)*CC(*O)+HO2=C5H8O3_Olef 3.35E10 0.600 -2105.6
DUP
C2H3+CC(C)*CC*O=C2H4+CC(CJ)*CC(*O) 7.46E12 0.000 9034.2
OH+CC(C)*CC*O=H2O+CC(CJ)*CC(*O) 7.80E5 2.300 -1362.3
C3H3+CC(C)*CC*O=C3H4-A+CC(CJ)*CC(*O) 1.32E13 0.000 22418.2
C5H9O2r_1=SC4H7OH-I+HCO 5.98E13 0.000 22896.2
CH3+CC(C)*CC*O=CH4+CC(CJ)*CC(*O) 7.68E12 0.000 13838.1
C5H7O2r_Olef=C5H6O2_Olef+H 1.17E10 1.000 18548.8
CC(C)*CC*O+CH3=C6H11Or 1.39E12 0.000 8293.3
DUP

CC (C) *CC*O+CH3=C6H11Or 1.39E12 0.000 8293.3
 DUP
 CC (CJ) *CC (*O)=C*C (CJ) CC*O 7.20E12 0.000 37929.3
 CC (C) *CC*O+H=CCJ (C) CC*O 9.27E13 0.000 4780.0
 CC (C) *CC*O+H=C5H9Or_2 1.62E13 0.000 4517.1
 C*C (C) CCJ (*O)=IC4H7+CO 3.30E12 0.620 17298.8
 C5H7O2r_olef=C*[C]CC*O+CH2O 2.70E14 0.000 23890.4
 C6H11Or=CC (C) *CC+HCO 8.10E13 0.000 20912.5
 CC (CJ) *CC (*O)+HO2=C*C (C) C (OOH) C*O 3.35E10 0.600 -2105.6
 DUP
 CC (CJ) *CC (*O)+HO2=C*C (C) C (OOH) C*O 3.35E10 0.600 -2105.6
 DUP
 C3H5-S+CC (C) *CC*O=C3H6+CC (CJ) *CC (*O) 7.46E12 0.000 9034.2
 H+CC (C) *CC*O=H2+CC (CJ) *CC (*O) 7.28E13 0.000 9177.6
 C5H8O3_olef_4=C5H7O2r_olef+OH 1.59E20 -1.500 42857.5
 C3H5-T+CC (C) *CC*O=C3H6+CC (CJ) *CC (*O) 5.53E12 0.000 10038.0
 HO2+CC (C) *CC*O=H2O2+CC (CJ) *CC (*O) 7.68E-2 4.400 13546.5
 C2H5+CC (C) *CC*O=C2H6+CC (CJ) *CC (*O) 1.25E12 0.000 15128.7
 C*C (CJ) CC*O=C3H4-A+CH2CHO 4.33E15 0.000 58674.5
 C5H7O2r_olef_4=C3H5-T+CHOCHO 8.10E14 0.000 23890.4
 C3H3+CC (C) *CC*O=C3H4-P+CC (CJ) *CC (*O) 4.40E12 0.000 22418.2
 CC (C) *CC*O+CH3=C6H11Or_2 5.62E11 0.000 8532.3

 C6H13r=C5H10_olef_1+CH3 9.32E13 0.000 30424.7
 CC (C) *CC+CH3=C6H13r_6 5.59E11 0.000 12428.0
 CH3+CC (C) C*C=CH4+CC5H9-A 3.10E13 0.000 17686.0
 C3H5-T+C5H10_olef_1=C3H6+C5H9r_olef_2 1.19E13 0.000 8365.0
 C5H11r_3=C5H11r_1 7.20E12 0.000 42733.2
 HO2+AC5H10=H2O2+AC5H9-C 5.12E-2 4.400 13546.5
 HO2+C5H10_olef_1=H2O2+C*CCJCC 7.68E-2 4.400 13546.5
 C3H5-A+AC5H10=C3H6+AC5H9-C 3.58E13 0.000 24425.8
 C5H10_olef_1+H=CCCJCC 6.75E13 0.000 4803.9
 C3H5-T+C5H10_olef_1=C3H6+C*CCJCC 5.53E12 0.000 10038.0
 C2H3+CC (C) *CC=C2H4+AC5H9-C 7.46E12 0.000 9034.2
 CH3+C5H10_olef_1=CH4+C*CCJCC 7.68E12 0.000 13838.1
 C3H3+CC (C) *CC=C3H4-A+AC5H9-C 8.80E12 0.000 22418.2
 NC3H7+C5H10_olef_1=C3H8+C5H9r_olef_3 3.33E12 0.000 18307.4
 C3H5-S+C5H10_olef_1=C3H6+C*CCJCC 7.46E12 0.000 9034.2
 NC3H7+AC5H10=C3H8+AC5H9-D 3.32E12 0.000 18307.4
 C6H13r_1=C3H6+IC3H7 6.88E13 0.000 26242.2
 C2H5+AC5H10=C2H6+AC5H9-D 4.98E12 0.000 18976.6
 C5H10_olef_1+H=CCJCCC 6.75E13 0.000 4803.9
 AC5H10+H=C5H11r 6.28E13 0.000 3250.4
 CH3+AC5H10=CH4+AC5H9-D 3.10E13 0.000 17686.0
 AC5H10+H=C5H11r_1 1.71E13 0.000 6190.1
 DUP
 CJCCCC=C2H4+NC3H7 5.05E13 0.000 28632.2
 HO2+CC (C) *CC=H2O2+B1E3M3J 7.68E-2 4.400 13546.5
 C3H5-A+AC5H10=C3H6+AC5H9-D 5.53E13 0.000 29946.7
 C5H11r_1=C2H5+C3H6 5.52E13 0.000 28536.6
 C3H3+CC (C) C*C=C3H4-A+CC5H9-A 4.56E13 0.000 26266.1
 C2H3+C5H10_olef_1=C2H4+C5H9r_olef_3 3.01E13 0.000 12882.1
 C3H3+AC5H10=C3H4-A+AC5H9-C 1.90E13 0.000 20745.2
 C2H3+AC5H10=C2H4+AC5H9-C 1.61E13 0.000 7361.2
 C3H3+AC5H10=C3H4-P+AC5H9-D 1.56E13 0.000 26266.1
 OH+C5H10_olef_1=H2O+C*CCJCC 7.80E5 2.300 -1362.3
 C3H3+C5H10_olef_1=C3H4-P+C5H9r_olef_3 1.60E13 0.000 26266.1
 C2H5+CC (C) *CC=C2H6+AC5H9-C 1.25E12 0.000 15128.7

IC3H7+AC5H10=C3H8+AC5H9-A2	1.60E12	0.000	15750.1
NC3H7+AC5H10=C3H8+AC5H9-C	1.78E12	0.000	12786.5
C3H5-S+AC5H10=C3H6+AC5H9-C	1.61E13	0.000	7361.2
IC3H7+AC5H10=C3H8+AC5H9-D	6.11E12	0.000	19598.0
C2H5+C5H10_olef_1=C2H6+C*CCJCC	1.25E12	0.000	15128.7
C3H3+CC(C)*C=C3H4-P+B1E3M3J3.15E12	1.15E12	0.000	19287.3
HO2+CC(C)*C=H2O2+B1E3M3J	2.56E-2	4.400	13546.5
OH+AC5H10=H2O+AC5H9-C	1.50E5	2.400	-932.1
CH3+CC(C)*C=CH4+B1E3M3J	5.50E12	0.000	10707.2
C3H5-T+CC(C)*C=C3H6+B1E3M3J3.96E12	3.96E12	0.000	6907.1
C3H5-S+C5H10_olef_1=C3H6+C5H9r_olef_2	1.61E13	0.000	7361.2
AC5H10+H=C5H11r_1	1.71E13	0.000	6190.1
DUP			
C5H11r_3=C4H8-2+CH3	9.32E13	0.000	30424.7
H+CC(C)*C=H2+CC5H9-A	3.51E14	0.000	12786.5
C3H3+AC5H10=C3H4-A+AC5H9-D	4.61E13	0.000	26266.1
C3H5-S+CC(C)*C=C3H6+B1E3M3J5.34E12	5.34E12	0.000	5903.3
CH3+AC5H10=CH4+AC5H9-A2	7.68E12	0.000	13838.1
C2H5+C5H10_olef_1=C2H6+C5H9r_olef_2	2.69E12	0.000	13455.7
C6H13r_4=C4H8-2+C2H5	3.35E13	0.000	28345.4
IC3H7+C5H10_olef_1=C3H8+C5H9r_olef_2	3.45E12	0.000	14077.1
NC3H7+CC(C)*CC=C3H8+B1E3M3J	8.25E11	0.000	14459.5
IC3H7+C5H10_olef_1=C3H8+C*CCJCC	1.60E12	0.000	15750.1
NC3H7+AC5H10=C3H8+AC5H9-A2	8.25E11	0.000	14459.5
C5H11r_4=C5H11r_1	9.00E11	0.000	25573.0
C3H5-T+C5H10_olef_1=C3H6+C5H9r_olef_3	2.23E13	0.000	13885.9
CC(C)*C+H=C5H11r_4	6.46E13	0.000	5377.5
C3H3+AC5H10=C3H4-P+AC5H9-A2	4.40E12	0.000	22418.2
CCCJCC=CH3+C4H8-1	8.54E13	0.000	30520.3
C3H5-S+CC(C)*C=C3H6+CC5H9-A3.01E13	3.01E13	0.000	12882.1
C3H5-A+CC(C)*C=C3H6+CC5H9-A5.47E13	5.47E13	0.000	29946.7
C5H11r_1=C5H11r_1	3.60E12	0.000	42111.8
C3H5-T+AC5H10=C3H6+AC5H9-C	1.19E13	0.000	8365.0
C5H11r_4=C2H4+IC3H7	6.30E13	0.000	26337.8
C3H3+CC(C)*C=C3H4-A+B1E3M3J6.30E12	6.30E12	0.000	19287.3
H+AC5H10=H2+AC5H9-A2	7.28E13	0.000	9177.6
IC3H7+AC5H10=C3H8+AC5H9-C	3.45E12	0.000	14077.1
C2H5+CC(C)*C=C2H6+B1E3M3J	8.92E11	0.000	11997.8
C3H3+C5H10_olef_1=C3H4-P+C5H9r_olef_2	9.49E12	0.000	20745.2
CH3+C5H10_olef_1=CH4+C5H9r_olef_3	3.10E13	0.000	17686.0
C3H5-S+CC(C)*CC=C3H6+AC5H9-C7.46E12	7.46E12	0.000	9034.2
NC3H7+CC(C)*C=C3H8+B1E3M3J	5.91E11	0.000	11328.6
CCJCCC=CJCCCC	9.00E11	0.000	26194.4
B13DE2MJ+CH3=B13DE2E	1.00E+13	0.000	0.00
OH+CC(C)*CC=H2O+AC5H9-C	7.80E5	2.300	-1362.3
H+CC(C)*C=H2+B1E3M3J	5.78E13	0.000	6190.1
CH3+CC(C)*CC=CH4+AC5H9-C	7.68E12	0.000	13838.1
C5H11r=CH3+IC4H8	4.62E13	0.000	30114.0
C3H5-T+CC(C)*C=C3H6+CC5H9-A2.23E13	2.23E13	0.000	13885.9
C2H5+AC5H10=C2H6+AC5H9-C	2.69E12	0.000	13455.7
H+AC5H10=H2+AC5H9-C	1.59E14	0.000	7361.2
NC3H7+C5H10_olef_1=C3H8+C5H9r_olef_2	1.78E12	0.000	12786.5
CH3+CC(C)*CC=CH4+B1E3M3J	7.68E12	0.000	13838.1
C6H13r_8=C2H5+IC4H8	1.56E13	0.000	28393.2
C2H3+CC(C)*C=C2H4+CC5H9-A	3.01E13	0.000	12882.1
C3H5-A+CC(C)*C=C3H6+B1E3M3J1.19E13	1.19E13	0.000	22967.9
C5H10_olef_1+CH3=C6H13r_4	8.89E11	0.000	11472.0
DUP			

H+CC(C)*CC=H2+AC5H9-C 7.28E13 0.000 9177.6
IC3H7+CC(C)*CC=C3H8+AC5H9-C 1.60E12 0.000 15750.1
C3H5-A+CC(C)*CC=C3H6+AC5H9-C 1.66E13 0.000 26098.8
CC(C)C*C+CH3=C6H13r 1.83E12 0.000 9966.3
C2H3+AC5H10=C2H4+AC5H9-A2 7.46E12 0.000 9034.2
C3H3+CC(C)*CC=C3H4-A+B1E3M3J 8.80E12 0.000 22418.2
C3H3+AC5H10=C3H4-A+AC5H9-A2 1.32E13 0.000 22418.2
OH+AC5H10=H2O+AC5H9-A2 7.80E5 2.300 -1362.3
AC5H10+CH3=C6H13r_8 1.13E12 0.000 12762.6
CC(C)C*C+CH3=C6H13r_1 9.02E11 0.000 11806.6
DUP
C2H3+C5H10_Olef_1=C2H4+C5H9r_Olef_2 1.61E13 0.000 7361.2
H+C5H10_Olef_1=H2+C5H9r_Olef_2 1.59E14 0.000 7361.2
OH+C5H10_Olef_1=H2O+C5H9r_Olef_2 1.50E5 2.400 -932.1
C3H5-S+AC5H10=C3H6+AC5H9-D 3.01E13 0.000 12882.1
NC3H7+C5H10_Olef_1=C3H8+C*CCJCC 8.25E11 0.000 14459.5
C2H5+CC(C)*CC=C2H6+B1E3M3J 1.25E12 0.000 15128.7
OH+CC(C)C*C=H2O+CC5H9-A 1.36E7 1.813 867.9
OH+C5H10_Olef_1=H2O+C5H9r_Olef_3 1.36E7 1.813 867.9
CH3+C5H10_Olef_1=CH4+C5H9r_Olef_2 1.66E13 0.000 12165.1
C5H11r_1=C4H8-1+CH3 7.68E13 0.000 30615.9
C3H5-S+C5H10_Olef_1=C3H6+C5H9r_Olef_3 3.01E13 0.000 12882.1
C3H5-A+AC5H10=C3H6+AC5H9-A2 1.66E13 0.000 26098.8
NC3H7+CC(C)*CC=C3H8+AC5H9-C 8.25E11 0.000 14459.5
C3H3+CC(C)*CC=C3H4-P+B1E3M3J 4.40E12 0.000 22418.2
C3H5-A+C5H10_Olef_1=C3H6+C5H9r_Olef_3 5.60E13 0.000 29946.7
H+CC(C)*CC=H2+B1E3M3J 7.28E13 0.000 9177.6
CC(C)*CC+CH3=C6H13r_5 2.22E12 0.000 11065.7
HO2+CC(C)*CC=H2O2+AC5H9-C 7.68E-2 4.400 13546.5
CJCCCC=CCJCC 4.80E12 0.000 39674.0
C3H3+C5H10_Olef_1=C3H4-P+C*CCJCC 4.40E12 0.000 22418.2
H+C5H10_Olef_1=H2+C5H9r_Olef_3 3.51E14 0.000 12786.5
C2H5+AC5H10=C2H6+AC5H9-A2 1.25E12 0.000 15128.7
C3H5-A+C5H10_Olef_1=C3H6+C*CCJCC 1.66E13 0.000 26098.8
C2H3+AC5H10=C2H4+AC5H9-D 3.01E13 0.000 12882.1
CC(C)*CC+H=C5H11r 7.62E13 0.000 4206.4
CC(C)C*C+CH3=C6H13r_1 9.02E11 0.000 11806.6
DUP
OH+CC(C)*CC=H2O+B1E3M3J 7.80E5 2.300 -1362.3
IC3H7+CC(C)*CC=C3H8+B1E3M3J 1.60E12 0.000 15750.1
HO2+AC5H10=H2O2+AC5H9-A2 7.68E-2 4.400 13546.5
C2H5+CC(C)C*C=C2H6+CC5H9-A 4.94E12 0.000 18976.6
IC3H7+C5H10_Olef_1=C3H8+C5H9r_Olef_3 6.28E12 0.000 19598.0
C5H10_Olef_1+CH3=C6H13r_4 8.89E11 0.000 11472.0
DUP
C3H5-T+CC(C)*CC=C3H6+B1E3M3J 5.53E12 0.000 10038.0
CH3+AC5H10=CH4+AC5H9-C 1.66E13 0.000 12165.1
C3H5-T+AC5H10=C3H6+AC5H9-D 2.23E13 0.000 13885.9
C3H5-T+AC5H10=C3H6+AC5H9-A2 5.53E12 0.000 10038.0
CC(C)*CC+H=C5H11r_3 1.79E13 0.000 5616.5
C3H3+C5H10_Olef_1=C3H4-A+C*CCJCC 1.32E13 0.000 22418.2
C2H3+CC(C)*CC=C2H4+B1E3M3J 7.46E12 0.000 9034.2
CC(C)C*C+H=C5H11r_3 5.56E13 0.000 3847.9
H+AC5H10=H2+AC5H9-D 3.51E14 0.000 12786.5
C3H3+AC5H10=C3H4-P+AC5H9-C 9.49E12 0.000 20745.2
HO2+C5H10_Olef_1=H2O2+C5H9r_Olef_2 5.12E-2 4.400 13546.5
IC3H7+CC(C)C*C=C3H8+CC5H9-A 6.05E12 0.000 19598.0
NC3H7+CC(C)C*C=C3H8+CC5H9-A 3.29E12 0.000 18307.4

CCJCCC=C3H6+C2H5 3.07E13 0.000 28441.0
 C2H3+CC(C)C*C=C2H4+B1E3M3J 5.34E12 0.000 5903.3
 H+C5H10_olef_1=H2+C*CCJCC 7.28E13 0.000 9177.6
 C2H5+C5H10_olef_1=C2H6+C5H9r_olef_3 5.03E12 0.000 18976.6
 C3H3+C5H10_olef_1=C3H4-A+C5H9r_olef_2 1.90E13 0.000 20745.2
 AC5H10+CH3=C6H13r_7 2.29E12 0.000 9560.0
 C5H11r_4=C5H11r 2.40E12 0.000 37929.3
 C3H3+CC(C)C*C=C3H4-P+CC5H9-A1.54E13 0.000 26266.1
 C3H5-A+CC(C)*CC=C3H6+B1E3M3J1.66E13 0.000 26098.8
 C3H3+CC(C)*CC=C3H4-P+AC5H9-C4.40E12 0.000 22418.2
 C3H5-T+CC(C)*CC=C3H6+AC5H9-C5.53E12 0.000 10038.0
 C3H3+C5H10_olef_1=C3H4-A+C5H9r_olef_3 4.75E13 0.000 26266.1
 OH+AC5H10=H2O+AC5H9-D 1.36E7 1.813 867.9
 C3H5-A+C5H10_olef_1=C3H6+C5H9r_olef_2 3.58E13 0.000 24425.8
 C3H5-S+AC5H10=C3H6+AC5H9-A2 7.46E12 0.000 9034.2
 C3H5-S+CC(C)*CC=C3H6+B1E3M3J7.46E12 0.000 9034.2
 C2H3+C5H10_olef_1=C2H4+C*CCJCC 7.46E12 0.000 9034.2
 IC3H7+CC(C)C*C=C3H8+B1E3M3J 1.14E12 0.000 12619.2
 H+HX15DE2V5M=H2+C9H13r_olef 1.59E14 0.000 7361.2
 HO2+C7H10_olef=H2O2+C7H9r_olef_1 5.12E-2 4.400 13546.5
 HO2+B13DE2E=H2O2+C6H9r_olef 5.12E-2 4.400 13546.5
 C3H5-S+B13DE2E=C3H6+C6H9r_olef_1 3.01E13 0.000 12882.1
 C3H3+C*(C)CCC*C=C3H4-P+C7H11r_olef_3 4.40E12 0.000 22418.2
 OH+C*(C)CCC*C=H2O+C7H11r_olef_3 7.80E5 2.300 -1362.3
 C7H13r_olef_3=C6H10+CH3 7.68E13 0.000 30615.9
 C3H3+C7H10_olef=C3H4-P+C7H9r_olef_1 1.02E13 0.000 18498.6
 C7H9r_olef_1=C6H6_olef+CH3 1.08E15 0.000 58674.5
 C8H11r_olef_3=C6H7r_olef_1+C2H4 7.81E13 0.000 34200.9
 C7H11r_olef_4=C6H8_olef_1+CH3 7.35E15 0.000 67421.9
 C8H11r_olef_4=C3H3+B13DE2M 1.06E14 0.000 38933.1
 H+C7H10_olef=H2+C7H9r_olef 12.01E14 0.000 6190.1
 OH+HX15DE2V5M=H2O+C9H13r_olef 1.50E5 2.400 -932.1
 C6H9r_olef_1=C4H5-I+C2H4 7.04E13 0.000 30711.5
 C10H15r_olef_3=C4H6+C6H9r_olef_1 3.06E13 0.000 25238.4
 C2H5+HX15DE2V5=C2H6+C10H13r_olef 5.38E12 0.000 13455.7
 C9H15r_olef=C4H612+AC5H9-D 5.28E15 0.000 65342.6
 C6H11r_olef(m1)=C2H3+C4H8-14.19E13 0.000 33149.3
 HX15DE2V5M+H=C9H15r_olef 5.03E13 0.000 2748.5
 C3H3+HX15DE2V=C3H4-A+C8H11r_olef_1 9.49E12 0.000 20745.2
 C3H3+B13DE2E=C3H4-P+C6H9r_olef 9.49E12 0.000 20745.2
 C10H13r_olef=C2H3+C8H10_olef 2.39E14 0.000 39458.9
 HX15DE2V+H=C8H13r_olef_6 2.53E13 0.000 6739.8
 DUP
 C3H3+HX15DE2V5M=C3H4-A+C9H13r_olef 2.85E13 0.000 20745.2
 C6H9r_olef=C2H3+C4H612 3.52E13 0.000 30711.5
 C8H13r_olef_4=C3H5-A+B13DE2M2.27E13 0.000 28966.8
 C3H3+C6H8_olef_1=C3H4-P+C6H7r_olef 1.02E13 0.000 18498.6
 C2H5+C7H10_olef=C2H6+C7H9r_olef 1.25E12 0.000 15128.7
 C3H5-A+HX15DE2V5M=C3H6+C9H13r_olef_2 1.66E13 0.000 26098.8
 C3H5-A+HX15DE2V=C3H6+C8H11r_olef_1 3.58E13 0.000 24425.8
 C2H5+C*(C)CCC*C=C2H6+C7H11r_olef_5 2.69E12 0.000 13455.7
 C6H11r_olef(m0)=C4H612+C2H5 7.77E14 0.000 56595.2
 C9H13r_olef=C2H3+C7H10_olef 3.52E13 0.000 30711.5
 C3H5-T+B13DE2E=C3H6+C6H9r_olef_1 2.23E13 0.000 13885.9
 HO2+C6H10=H2O2+C6H9-A 1.02E-1 4.400 13546.5
 C3H3+C7H10_olef=C3H4-P+C7H9r_olef 4.40E12 0.000 22418.2
 HX15DE2V+H=C8H13r_olef_6 2.53E13 0.000 6739.8
 DUP

HO2+C6H8_olef_1=H2O2+C6H7r_olef	5.12E-2	4.400	13546.5
HX15DE2V+H=C8H13r_olef_4	5.61E13	0.000	2294.4
C8H11r_olef_2=C4H5-I+C4H612	1.08E15	0.000	58674.5
OH+B13DE2E=H2O+C6H9r_olef	1.50E5	2.400	-932.1
B13DE2E+H=C6H11r_olef_(ml)	2.53E13	0.000	6739.8
DUP			
C3H5-S+C7H10_olef=C3H6+C7H9r_olef	7.46E12	0.000	9034.2
C2H5+B13DE2E=C2H6+C6H9r_olef	2.69E12	0.000	13455.7
C8H13r_olef_2=C4H71-4+C4H6125	2.28E15	0.000	65342.6
HX15DE2V5M+H=C9H15r_olef_1	7.85E13	0.000	5951.1
C7H13r_olef_3=C4H71-4+C3H6	5.52E13	0.000	28536.6
C3H3+B13DE2E=C3H4-P+C6H9r_olef_1	1.56E13	0.000	26266.1
OH+HX15DE2V=H2O+C8H11r_olef_1	1.50E5	2.400	-932.1
C3H3+HX15DE2V=C3H4-P+C8H11r_olef	9.49E12	0.000	20745.2
C2H3+C*(C)CCC*C=C2H4+C7H11r_olef_3	7.46E12	0.000	9034.2
OH+C*(C)CCC*C=H2O+C7H11r_olef_5	1.50E5	2.400	-932.1
C3H3+C7H10_olef=C3H4-A+C7H9r_olef_1	3.07E13	0.000	18498.6
C6H10+H=C*CCCCJC	1.11E14	0.000	3847.9
C9H15r_olef_1=C2H4+H15DE2M-T	7.81E13	0.000	34200.9
C3H5-T+HX15DE25V=C3H6+C10H13r_olef	2.38E13	0.000	8365.0
C2H5+C*(C)CCC*C=C2H6+C7H11r_olef_3	1.25E12	0.000	15128.7
C3H5-S+HX15DE2V=C3H6+C8H11r_olef_1	1.61E13	0.000	7361.2
C9H13r_olef_1=C8H10_olef+CH3	1.08E15	0.000	58674.5
HO2+HX15DE2V=H2O2+C8H11r_olef_1	5.12E-2	4.400	13546.5
HX15DE25V+H=C10H15r_olef_2	1.12E14	0.000	2294.4
HX15DE2V5M+H=C9H15r_olef_6	2.53E13	0.000	6739.8
DUP			
C3H5-S+C*(C)CCC*C=C3H6+C7H11r_olef_3	7.46E12	0.000	9034.2
C3H5-S+C7H10_olef=C3H6+C7H9r_olef_1	1.73E13	0.000	5114.6
C2H5+HX15DE2V=C2H6+C8H11r_olef_1	2.69E12	0.000	13455.7
C2H3+C7H10_olef=C2H4+C7H9r_olef	7.46E12	0.000	9034.2
CH3+HX15DE2V5M=CH4+C9H13r_olef	1.66E13	0.000	12165.1
C7H13r_olef=C3H6+IC4H7	9.15E12	0.000	20554.0
CH3+B13DE2E=CH4+C6H9r_olef	13.10E13	0.000	17686.0
C9H13r_olef=C6H8_olef+C3H5-T	2.65E14	0.000	42948.3
H+HX15DE2V=H2+C8H11r_olef_1	1.59E14	0.000	7361.2
CH3+C*(C)CCC*C=CH4+C7H11r_olef_4	1.66E13	0.000	12165.1
C3H5-A+B13DE2E=C3H6+C6H9r_olef	3.58E13	0.000	24425.8
C8H10_olef+H=C8H11r_olef_2	5.03E13	0.000	2748.5
C3H5-T+C*(C)CCC*C=C3H6+C7H11r_olef_3	5.53E12	0.000	10038.0
C3H5-T+C8H10_olef=C3H6+C8H9r_olef	1.28E13	0.000	6118.4
C3H5-T+C7H10_olef=C3H6+C7H9r_olef_1	1.28E13	0.000	6118.4
C3H5-S+C8H10_olef=C3H6+C8H9r_olef	1.73E13	0.000	5114.6
C3H3+C*(C)CCC*C=C3H4-P+C7H11r_olef_5	9.49E12	0.000	20745.2
C6H9r_olef_3=C2H3+C4H6	1.39E14	0.000	36543.1
C3H5-A+C6H10=C3H6+C6H9-A	7.15E13	0.000	24425.8
HO2+HX15DE2V5M=H2O2+C9H13r_olef_2	7.68E-2	4.400	13546.5
C3H5-A+C8H10_olef=C3H6+C8H9r_olef	3.85E13	0.000	22179.2
C9H15r_olef_4=HX15DE2V+CH3	7.68E13	0.000	30615.9
C3H3+HX15DE2V5M=C3H4-A+C9H13r_olef_2	4.40E12	0.000	22418.2
OH+C*(C)CCC*C=H2O+C7H11r_olef_4	1.50E5	2.400	-932.1
C3H3+HX15DE2V5M=C3H4-P+C9H13r_olef	9.49E12	0.000	20745.2
C2H5+HX15DE2V=C2H6+C8H11r_olef	2.69E12	0.000	13455.7
C3H5-A+C*(C)CCC*C=C3H6+C7H11r_olef_5	3.58E13	0.000	24425.8
C3H5-A+C6H8_olef_1=C3H6+C6H7r_olef	3.85E13	0.000	22179.2
C3H5-A+HX15DE25V=C3H6+C10H13r_olef	7.15E13	0.000	24425.8
CH3+C6H8_olef_1=CH4+C6H7r_olef	1.78E13	0.000	9918.5
C3H5-A+C7H10_olef=C3H6+C7H9r_olef_1	3.85E13	0.000	22179.2

C3H5-A+C*(C)CCC*C=C3H6+C7H11r_Olef_3 1.66E13 0.000 26098.8
C6H9r_Olef_5=C2H4+C4H5-I 1.51E13 0.000 20745.2
C3H5-T+C*(C)CCC*C=C3H6+C7H11r_Olef_5 1.19E13 0.000 8365.0
C2H3+C*(C)CCC*C=C2H4+C7H11r_Olef_5 1.61E13 0.000 7361.2
C8H11r_Olef_6=C6H8_Olef_1+C2H3 4.19E13 0.000 33149.3
H+C7H10_Olef=H2+C7H9r_Olef 7.28E13 0.000 9177.6
C6H9r_Olef_4=C3H3+C3H6 4.27E13 0.000 30520.3
B13DE2E+H=C6H11r_Olef_1 7.85E13 0.000 5951.1
C2H3+HX15DE2V5M=C2H4+C9H13r_Olef_1 1.61E13 0.000 7361.2
HX15DE2V+H=C8H13r_Olef_3 7.85E13 0.000 5951.1
B13DE2E+H=C6H11r_Olef_(m1) 2.53E13 0.000 6739.8
DUP
C3H3+HX15DE2V=C3H4-A+C10H13r_Olef 1.90E13 0.000 20745.2
C2H3+HX15DE2V5M=C2H4+C9H13r_Olef 1.61E13 0.000 7361.2
C8H13r_Olef_3=C*CJCCC*C+C2H4 7.81E13 0.000 34200.9
OH+HX15DE2V=H2O+C8H11r_Olef 1.50E5 2.400 -932.1
C7H11r_Olef_3=C4H71-4+C3H4-A3.11E15 0.000 56595.2
C9H15r_Olef_4=C6H9r_Olef_1+C3H6 5.52E13 0.000 28536.6
C7H11r_Olef_4=C2H3+B13DE2M 2.35E14 0.000 45290.5
H+C*(C)CCC*C=H2+C7H11r_Olef_4 1.59E14 0.000 7361.2
C7H11r_Olef=C3H3+IC4H8 4.62E13 0.000 30114.0
C10H15r_Olef_3=C2H3+HX15DE2V4.19E13 0.000 33149.3
C3H5-T+B13DE2E=C3H6+C6H9r_Olef 1.19E13 0.000 8365.0
CH3+C7H10_Olef=CH4+C7H9r_Olef 7.68E12 0.000 13838.1
C*(C)CCC*C+H=C7H13r_Olef_1 6.46E13 0.000 5377.5
C2H3+C8H10_Olef=C2H4+C8H9r_Olef 1.73E13 0.000 5114.6
C9H15r_Olef_6=C4H6+AC5H9-D 3.06E13 0.000 25238.4
C2H5+C*(C)CCC*C=C2H6+C7H11r_Olef_4 2.69E12 0.000 13455.7
C10H13r_Olef=C6H8_Olef+C4H5-I 2.39E14 0.000 39458.9
C2H3+HX15DE2V=C2H4+C8H11r_Olef 1.61E13 0.000 7361.2
C9H15r_Olef_5=B13DE2M+IC4H7 2.27E13 0.000 28966.8
CH3+C*(C)CCC*C=CH4+C7H11r_Olef_3 7.68E12 0.000 13838.1
H+C*(C)CCC*C=H2+C7H11r_Olef_5 1.59E14 0.000 7361.2
C3H3+HX15DE2V=C3H4-A+C8H11r_Olef 9.49E12 0.000 20745.2
C3H5-T+HX15DE2V5M=C3H6+C9H13r_Olef 1.19E13 0.000 8365.0
C2H5+HX15DE2V5M=C2H6+C9H13r_Olef 2.69E12 0.000 13455.7
C6H8_Olef+H=C6H9r_Olef_2 1.01E14 0.000 1696.9
C8H10_Olef+H=C8H11r_Olef_4 5.61E13 0.000 2294.4
C2H5+HX15DE2V5M=C2H6+C9H13r_Olef_2 1.25E12 0.000 15128.7
C8H13r_Olef_6=C4H71-4+C4H6 3.06E13 0.000 25238.4
C7H11r_Olef_1=C4H5-I+C3H6 1.65E13 0.000 20649.6
HX15DE2V5M+H=C9H15r_Olef_6 2.53E13 0.000 6739.8
DUP
C6H10+H=C*CCCCCJ 1.29E14 0.000 5377.5
HO2+C*(C)CCC*C=H2O2+C7H11r_Olef_5 5.12E-2 4.400 13546.5
HX15DE25V+H=C10H15r_Olef_3 5.06E13 0.000 6739.8
DUP
CH3+C8H10_Olef=CH4+C8H9r_Olef 1.78E13 0.000 9918.5
C3H5-S+C6H8_Olef_1=C3H6+C6H7r_Olef 1.73E13 0.000 5114.6
H+C*(C)CCC*C=H2+C7H11r_Olef_3 7.28E13 0.000 9177.6
C8H10_Olef+H=C8H11r_Olef_6 2.53E13 0.000 6739.8
DUP
CH3+HX15DE2V5M=CH4+C9H13r_Olef_1 1.66E13 0.000 12165.1
C10H15r_Olef=C6H9r_Olef_1+C4H612 5.28E15 0.000 65342.6
C3H3+C7H10_Olef=C3H4-A+C7H9r_Olef 4.40E12 0.000 22418.2
CC(C)*CCJ(*O)=IC4H7-I1+CO 1.43E+15 0.115 26627
CC(C)*CC*O=IC4H8+CO 3.16E+130.00 59512
C7H10_Olef+H=C7H11r_Olef 6.28E13 0.000 3250.4

C8H10_Olef+H=C8H11r_Olef_3 7.85E13 0.000 5951.1
C*CCCCJ=C4H71-4+C2H4 5.05E13 0.000 28632.2
C6H8_Olef+H=C6H9r_Olef_1 1.57E14 0.000 5951.1
C3H5-T+C*(C)CCC*C=C3H6+C7H11r_Olef_4 1.19E13 0.000 8365.0
C8H13r_Olef_6=C6H10+C2H3 4.19E13 0.000 33149.3
CH3+C7H10_Olef=CH4+C7H9r_Olef_1 1.78E13 0.000 9918.5
C7H11r_Olef_1=C6H8_Olef_1+CH3 7.68E13 0.000 30615.9
C8H9r_Olef=C6H6_Olef+C2H3 3.52E13 0.000 30711.5
C9H13r_Olef_2=C6H9r_Olef_1+C3H4-A 3.11E15 0.000 56595.2
C3H5-T+HX15DE2V=C3H6+C8H11r_Olef 1.19E13 0.000 8365.0
C3H5-T+HX15DE2V=C3H6+C8H11r_Olef_1 1.19E13 0.000 8365.0
HX15DE2V5M+H=C9H15r_Olef_4 1.71E13 0.000 6190.1
DUP
C3H3+C8H10_Olef=C3H4-P+C8H9r_Olef 1.02E13 0.000 18498.6
C7H13r_Olef_1=C2H4+AC5H9-D 5.05E13 0.000 28632.2
C9H15r_Olef_2=B13DE2MJ+IC4H89.90E12 0.000 20147.7
CH3+HX15DE2V=CH4+C8H11r_Olef_1 1.66E13 0.000 12165.1
C6H9-A=C4H6+C2H3 2.35E14 0.000 45290.5
C3H3+HX15DE2V=C3H4-P+C8H11r_Olef_1 9.49E12 0.000 20745.2
C9H13r_Olef_1=C4H5-I+B13DE2M2.39E14 0.000 39458.9
C6H11r_Olef_(m1)=C4H6+C2H5 3.06E13 0.000 25238.4
C3H3+C6H10=C3H4-P+C6H9-A 1.90E13 0.000 20745.2
HO2+C8H10_Olef=H2O2+C8H9r_Olef 5.12E-2 4.400 13546.5
C2H3+HX15DE2V=C2H4+C8H11r_Olef_1 1.61E13 0.000 7361.2
C9H15r_Olef_6=C2H3+C*(C)CCC*C 4.19E13 0.000 33149.3
CH3+C6H10=CH4+C6H9-A 3.31E13 0.000 12165.1
HO2+HX15DE2V5M=H2O2+C9H13r_Olef 5.12E-2 4.400 13546.5
HO2+C7H10_Olef=H2O2+C7H9r_Olef 7.68E-2 4.400 13546.5
C2H3+HX15DE2V=C2H4+C10H13r_Olef 3.22E13 0.000 7361.2
HO2+C*(C)CCC*C=H2O2+C7H11r_Olef_4 5.12E-2 4.400 13546.5
C3H5-A+C*(C)CCC*C=C3H6+C7H11r_Olef_4 3.58E13 0.000 24425.8
C7H9r_Olef=C4H5-I+C3H4-A 1.08E15 0.000 58674.5
C8H11r_Olef_1=C6H8_Olef_1+C2H3 3.52E13 0.000 30711.5
C2H3+B13DE2E=C2H4+C6H9r_Olef_1 3.01E13 0.000 12882.1
C3H3+C*(C)CCC*C=C3H4-A+C7H11r_Olef_3 4.40E12 0.000 22418.2
H+C8H10_Olef=H2+C8H9r_Olef 2.01E14 0.000 6190.1
C3H5-A+HX15DE2V=C3H6+C8H11r_Olef 3.58E13 0.000 24425.8
C3H5-T+HX15DE2V5M=C3H6+C9H13r_Olef_2 5.53E12 0.000 10038.0
HX15DE2V5M+H=C10H15r_Olef_3 5.06E13 0.000 6739.8
DUP
C3H5-S+C*(C)CCC*C=C3H6+C7H11r_Olef_4 1.61E13 0.000 7361.2
OH+C7H10_Olef=H2O+C7H9r_Olef 7.80E5 2.300 -1362.3
C3H5-A+B13DE2E=C3H6+C6H9r_Olef_1 5.53E13 0.000 29946.7
C3H3+C6H10=C3H4-A+C6H9-A 1.90E13 0.000 20745.2
C3H3+HX15DE2V=C3H4-P+C10H13r_Olef 1.90E13 0.000 20745.2
C3H3+HX15DE2V5M=C3H4-P+C9H13r_Olef_1 9.49E12 0.000 20745.2
C3H5-S+C6H10=C3H6+C6H9-A 3.22E13 0.000 7361.2
C6H8_Olef+H=C6H9r_Olef 1.01E14 0.000 2748.5
C2H5+HX15DE2V5M=C2H6+C9H13r_Olef_1 2.69E12 0.000 13455.7
C3H3+C*(C)CCC*C=C3H4-P+C7H11r_Olef_4 9.49E12 0.000 20745.2
C3H5-A+C7H10_Olef=C3H6+C7H9r_Olef 1.66E13 0.000 26098.8
C3H5-S+HX15DE2V5M=C3H6+C9H13r_Olef_2 7.46E12 0.000 9034.2
C2H5+C8H10_Olef=C2H6+C8H9r_Olef 2.89E12 0.000 11209.1
C7H11r_Olef_5=C4H6+C3H5-T 2.65E14 0.000 42948.3
C2H3+C*(C)CCC*C=C2H4+C7H11r_Olef_4 1.61E13 0.000 7361.2
C3H5-A+HX15DE2V5M=C3H6+C9H13r_Olef_1 3.58E13 0.000 24425.8
HX15DE2V5M+H=C10H15r_Olef_1 1.57E14 0.000 5951.1
C3H5-S+HX15DE2V=C3H6+C10H13r_Olef 3.22E13 0.000 7361.2

C10H15r_Olef_1=C8H11r_Olef_7+C2H4 7.81E13 0.000 34200.9
C3H5-S+HX15DE2V5M=C3H6+C9H13r_Olef 1.61E13 0.000 7361.2
C3H3+HX15DE2V5M=C3H4-P+C9H13r_Olef_2 4.40E12 0.000 22418.2
C3H5-S+B13DE2E=C3H6+C6H9r_Olef 1.61E13 0.000 7361.2
B13DE2E+H=C6H11r_Olef_3 5.61E13 0.000 2294.4
C2H3+C6H8_Olef_1=C2H4+C6H7r_Olef 1.73E13 0.000 5114.6
C2H5+C7H10_Olef=C2H6+C7H9r_Olef_1 2.89E12 0.000 11209.1
C2H5+B13DE2E=C2H6+C6H9r_Olef_1 4.98E12 0.000 18976.6
HX15DE2V5M+H=C9H15r_Olef_5 5.61E13 0.000 2294.4
HO2+HX15DE25V=H2O2+C10H13r_Olef 1.02E-1 4.400 13546.5
C5H10O2_2+HOCHO=CC(C)(OH)CCHO+HOCHO 2.810E-002 3.286 -4509.0
C3H5-S+HX15DE2V5M=C3H6+C9H13r_Olef_1 1.61E13 0.000 7361.2
C3H5-T+HX15DE2V5M=C3H6+C9H13r_Olef_1 1.19E13 0.000 8365.0
C3H3+HX15DE2V5M=C3H4-A+C9H13r_Olef_1 2.85E13 0.000 20745.2
OH+HX15DE2V5M=H2O+C9H13r_Olef_1 1.50E5 2.400 -932.1
HX15DE2V+H=C8H13r_Olef_2 5.03E13 0.000 2748.5
C8H11r_Olef_1=C2H3+C6H8_Olef 2.35E14 0.000 45290.5
B13DE2E+H=C6H11r_Olef(m0) 5.03E13 0.000 2748.5
HO2+C*(C)CCC*C=H2O2+C7H11r_Olef_3 7.68E-2 4.400 13546.5
C2H3+C6H10=C2H4+C6H9-A 3.22E13 0.000 7361.2
OH+HX15DE2V5M=H2O+C9H13r_Olef_2 7.80E5 2.300 -1362.3
C8H13r_Olef_1=C2H4+C6H9r_Olef_1 5.05E13 0.000 28632.2
C2H5+C6H10=C2H6+C6H9-A 5.38E12 0.000 13455.7
HX15DE2V+H=C8H13r_Olef_1 6.46E13 0.000 5377.5
HX15DE2V5M+H=C9H15r_Olef_2 6.28E13 0.000 3250.4
C*(C)CCC*C+H=C7H13r_Olef 5.56E13 0.000 3847.9
C3H3+C*(C)CCC*C=C3H4-A+C7H11r_Olef_4 2.85E13 0.000 20745.2
CH3+HX15DE25V=CH4+C10H13r_Olef 3.31E13 0.000 12165.1
C3H3+C*(C)CCC*C=C3H4-A+C7H11r_Olef_5 2.85E13 0.000 20745.2
C6H8_Olef+H=C6H9r_Olef_3 6.78E13 0.000 7456.8
B13DE2MJ+B13DE2MJ=HX15DE25V 1.00E+13 0.00 0.00
C3H5-S+HX15DE2V=C3H6+C8H11r_Olef 1.61E13 0.000 7361.2
H+C6H10=H2+C6H9-A 3.18E14 0.000 7361.2
C3H3+B13DE2E=C3H4-A+C6H9r_Olef 2.85E13 0.000 20745.2
C3H5-T+C7H10_Olef=C3H6+C7H9r_Olef 5.53E12 0.000 10038.0
C3H3+C8H10_Olef=C3H4-A+C8H9r_Olef 1.02E13 0.000 18498.6
C7H13r_Olef_2=C3H5-A+IC4H8 9.90E12 0.000 20147.7
H+B13DE2E=H2+C6H9r_Olef 1.59E14 0.000 7361.2
H+HX15DE2V=H2+C8H11r_Olef 1.59E14 0.000 7361.2
H+HX15DE2V5M=H2+C9H13r_Olef_2 7.28E13 0.000 9177.6
HO2+HX15DE2V5M=H2O2+C9H13r_Olef_1 5.12E-2 4.400 13546.5
C7H10_Olef+H=C7H11r_Olef_1 1.71E13 0.000 6190.1
DUP
C2H5+C6H8_Olef_1=C2H6+C6H7r_Olef 2.89E12 0.000 11209.1
H+B13DE2E=H2+C6H9r_Olef_1 3.51E14 0.000 12786.5
C8H13r_Olef=C3H6+B13DE2MJ 9.15E12 0.000 20554.0
C3H3+C6H8_Olef_1=C3H4-A+C6H7r_Olef 1.02E13 0.000 18498.6
H+HX15DE2V5M=H2+C9H13r_Olef_1 1.59E14 0.000 7361.2
C3H5-A+HX15DE2V5M=C3H6+C9H13r_Olef 3.58E13 0.000 24425.8
OH+C6H10=H2O+C6H9-A 3.00E5 2.400 -932.1
C2H3+B13DE2E=C2H4+C6H9r_Olef 1.61E13 0.000 7361.2
C8H10_Olef+H=C8H11r_Olef_6 2.53E13 0.000 6739.8
DUP
C3H5-S+C*(C)CCC*C=C3H6+C7H11r_Olef_5 1.61E13 0.000 7361.2
C8H11r_Olef_6=C4H5-I+C4H6 9.13E12 0.000 17351.4
C6H8_Olef_1+H=C6H9r_Olef_4 5.56E13 0.000 3847.9
HX15DE25V+H=C10H15r_Olef 1.01E14 0.000 2748.5
C5H10O2_2+H=CC(C)(OH)CCHO+H 5.55E+13 0.00 10950

C2H3+HX15DE2V5M=C2H4+C9H13r_Olef_2 7.46E12 0.000 9034.2
HX15DE2V+H=C8H13r_Olef 5.56E13 0.000 3847.9
C*CCCCJC=C3H5-A+C3H6 9.15E12 0.000 20554.0
C3H5-T+C6H10=C3H6+C6H9-A 2.38E13 0.000 8365.0
C8H11r_Olef=C4H6+C4H5-I 2.39E14 0.000 39458.9
C*(C)CCC*C+H=C7H13r_Olef_3 1.71E13 0.000 6190.1
DUP
OH+HX15DE25V=H2O+C10H13r_Olef 3.00E5 2.400 -932.1
C10H15r_Olef_2=B13DE2MJ+B13DE2M 2.27E13 0.000 28966.8
CH3+HX15DE2V5M=CH4+C9H13r_Olef_2 7.68E12 0.000 13838.1
C*(C)CCC*C+H=C7H13r_Olef_3 1.71E13 0.000 6190.1
DUP
C2H3+C7H10_Olef=C2H4+C7H9r_Olef_1 1.73E13 0.000 5114.6
HO2+HX15DE2V=H2O2+C8H11r_Olef 5.12E-2 4.400 13546.5
C3H5-T+C6H8_Olef_1=C3H6+C6H7r_Olef 1.28E13 0.000 6118.4
H+HX15DE25V=H2+C10H13r_Olef 3.18E14 0.000 7361.2
C*(C)CCC*C+H=C7H13r_Olef_2 6.28E13 0.000 3250.4
H+C6H8_Olef_1=H2+C6H7r_Olef 2.01E14 0.000 6190.1
HX15DE2V5M+H=C9H15r_Olef_4 1.71E13 0.000 6190.1
DUP
CH3+C*(C)CCC*C=CH4+C7H11r_Olef_5 1.66E13 0.000 12165.1
C7H10_Olef+H=C7H11r_Olef_1 1.71E13 0.000 6190.1
DUP
CH3+B13DE2E=CH4+C6H9r_Olef 1.66E13 0.000 12165.1
C6H11r_Olef_1=C2H4+C4H71-2 7.81E13 0.000 34200.9
C6H8_Olef_1+H=C6H9r_Olef_5 6.46E13 0.000 5377.5
C3H3+B13DE2E=C3H4-A+C6H9r_Olef_1 1.54E13 0.000 26266.1
CH3+HX15DE2V=CH4+C8H11r_Olef 1.66E13 0.000 12165.1
C4H5-I+Prenol=C4H6+C*(C)CJCOH 3.75E12 0.000 16849.5
C4H5-I+Prenol=C4H612+C*(C)CJCOH 8.29E12 0.000 26098.8
C4H5-I+Prenol=C4H6+CC(C)*CCJOH 8.10E12 0.000 15176.5
C4H5-I+Prenol=C4H612+CC(C)*CCJOH 1.79E13 0.000 24425.8
C2H3COCH3+H=CH2CH2COCH3 7.85E13 0.000 5951.1
C2H3COCH3+H=CH3CHCOCH3 5.03E13 0.000 2748.5
C2H5COCH2=CH3CHCOCH3 2.40E12 0.000 40606.1
CH2CH2COCH3=C2H5COCH2 9.00E11 0.000 23350.3
OH+CC(C)*CC*O=H2O+CC(C)*CCJ(*O) 9.24E+06 1.500 -962
IC3H5CHO+OH=IC3H5CO+H2O 2.69E+10 0.76 -340
CC(CJ)*CC(*O)=CC(C)*CCJ(*O) 1.50E+11 0.000 30663.7
IC4H7-I1=C3H4-P+CH3 5.00E+14 0.000 35540
B2E2M1OJ=>B13DE2M+OH 4.44E+11 0.000 7821
B2E3M1OJ=>B13DE2M+OH 4.44E+11 0.000 7821
C4H6O_Olef_5+HO2=C2H3COCH3+HO2 1.49E+05 1.67 6810
C4H6O_Olef_5+HOCHO=C2H3COCH3+HOCHO 2.81E-02 3.286 -4509
C4H6O_Olef_5=C2H3COCH3 8.59E+11 0.318 55900
CC(C)*CCOJ=C*(C)CJCOH 4.47E+05 1.51 619
CC(C)*CCOJ=IC4H7-I1+CH2O 2.70E+14 0.00 23892
CC(C)*CCOJ=CC(C)*CC*O+H 1.17E+10 1.00 18549
C4H612+CH3=AC5H9-C 40210 2.52 8847
C4H6O_Olef+CH3=C*(C)CJCOH 40210 2.52 8847

!*****
!***Isobutene oxidation mechanism***
!*****

!REF:2 PARAMETER FIT TO HONG ET AL.PROC. OF THE COMB. INST. 33 (2011)
309-316

H+O2<=>O+OH 15286.0	1.040E+014	0.000
!REF:SUTHERLAND ET AL., 21ST SYMPOSIUM, P. 929 (1986)		
O+H2<=>H+OH 6292.0	5.080E+004	2.670
!REF:LAM ET AL. SUBMITTED IJCK		
OH+H2<=>H+H2O 6990.0	4.380E+013	0.000
!FIT FROM NGUYEN JPCA 2013 HIGH PRESSURE LIMIT		
O+H2O<=>OH+OH 14986.8	6.70E+07	1.704
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
H2+M<=>H+H+M 104400.0	4.577E+019	-1.400
H2/ 2.50/ H2O/ 12.00/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/ C2H6/ 3.00/		
O+O+M<=>O2+M 0.0	6.165E+015	-0.500
H2/ 2.50/ H2O/ 12.00/ AR/ 0.83/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/ C2H6/ 3.00/		
O+H+M<=>OH+M 0.0	4.714E+018	-1.000
H2/ 2.50/ H2O/ 12.00/ AR/ 0.75/ CO/ 1.50/ CO2/ 2.00/ HE/ 0.75/ CH4/ 2.00/ C2H6/ 3.00/		
!REF: LI IJCK 36: 566-575, 2004		
!REF:OPTIMISED TO FIT H2 AND CH4 FLAMES DATA		
H+OH+M<=>H2O+M 0.0	3.500E+022	-2.000
!REF:EFFICIENCIES FROM GRI 3.0		
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/		
!REF:FERNANDES PCCP 2008		
H+O2(+M)<=>HO2(+M) 0.0	4.650E+012	0.440
LOW/ 0.0/	1.737E+019	-1.230
TROE/ 6.700E-001 1.000E-030 1.000E+030 1.000E+030/ H2/ 1.30/ CO/ 1.90/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/ C2H6/ 3.00/		
H+O2(+CO2)<=>HO2(+CO2) 1.116E+13 0.44 0.0 !		
LOW/ 8.82E+19 -1.4 0.0/		
TROE/ 6.700E-001 1.000E-030 1.000E+030 1.000E+030/		
H+O2(+AR)<=>HO2(+AR) 0.0	4.650E+012	0.440
!REF: BATES ET AL. PCCP 3 (2001) 2337-2342		
LOW/ 0.0/	6.810E+018	-1.200
TROE/ 7.000E-001 1.000E-030 1.000E+030 1.000E+030/		

!REF:LPL * 1.5 AK			
H+O2 (+HE) <=>HO2 (+HE)	4.650E+012	0.440	
0.0			
LOW/	9.192E+018	-1.200	
0.0/			
TROE/ 5.900E-001 1.000E-030 1.000E+030 1.000E+030/			
HO2+H<=>OH+OH	7.079E+013	0.000	
295.0			
!REF:MICHAEL SUTHERLAND 2000			
H2+O2<=>H+HO2	5.176E+005	2.433	
53502.0			
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)			
HO2+O<=>OH+O2	3.250E+013	0.000	
0.0			
!REF:HONG PCI 2013 1015C			
HO2+OH<=>H2O+O2	7.00E+12	0.0	
-1092.96			
DUP			
HO2+OH<=>H2O+O2	4.50E+14	0.0	
10929.6			
DUP			
!REF:HONG PCI 2013, KAPEL 2002			
HO2+HO2<=>H2O2+O2	1.00E+14	0.000	
11040.9			
DUP			
HO2+HO2<=>H2O2+O2	1.90E+11	0.000	-
1408.9			
DUP			
!REF:TROE, COMBUST. FLAME, 158:594-601 (2011)			
!REF:RATE CONSTANT IS FOR N2			
H2O2 (+H2O) <=>OH+OH (+H2O)	2.000E+012	0.900	
48749.0			
LOW/	1.865E+025	-2.300	
48749.0/			
TROE/ 5.100E-001 1.000E-030 1.000E+030/			
H2O2 (+M) <=>OH+OH (+M)	2.000E+012	0.900	
48749.0			
LOW/	2.490E+024	-2.300	
48749.0/			
TROE/ 4.300E-001 1.000E-030 1.000E+030/			
H2O/ 0.00/ CO2/ 1.60/ N2/ 1.50/ O2/ 1.20/ HE/ 0.65/ H2O2/ 7.70/			
!REF:EFFICIENCIES FOR H2 AND CO TAKEN FROM LI ET AL., INT. J. CHEM.			
KINET. 36:566-575 (2004)			
H2/ 3.70/ CO/ 2.80/			
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)			
H2O2+H<=>H2O+OH	2.410E+013	0.000	
3970.0			

!REF: ELLINGSON J. PHYS. CHEM. (2007) 111, (51), 13554-13566
 H2O2+H<=>H2+HO2 2.150E+010 1.000
 6000.0

!REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
 H2O2+O<=>OH+HO2 9.550E+006 2.000
 3970.0

!REF: HONG ET AL. J. PHYS. CHEM. A 114 (2010) 5718-5727
 H2O2+OH<=>H2O+HO2 1.740E+012 0.000
 318.0
 DUP
 H2O2+OH<=>H2O+HO2 7.590E+013 0.000
 7269.0
 DUP

!REF: MEULLER 99 * 0.76
 CO+O(+M)<=>CO2(+M) 1.362E+010 0.000
 2384.0
 LOW/ 1.173E+024 -2.790
 4191.0/
 H2/ 2.00/ H2O/ 12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/ HE/ 0.70/

!REF: 86TSA/ HAM * 0.44
 CO+O2<=>CO2+O 1.119E+012 0.000
 47700.0

!REF: JOSHI AND WANG IJCK (2006), 38, (1), 57-73.
 CO+OH<=>CO2+H 7.015E+004 2.053
 -355.7
 DUP
 CO+OH<=>CO2+H 5.757E+012 -0.664
 331.8
 DUP

!REF: YOU ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042
 CO+HO2<=>CO2+OH 1.570E+005 2.180
 17940.0

!REF: LI ET AL. IJCK 2007 *1.2
 HCO+M<=>H+CO+M 5.700E+011 0.660
 14870.0
 H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/

!REF: TIMONEN ET AL., JPC, 92:651 (1988)
 HCO+O2<=>CO+HO2 7.580E+012 0.000
 410.0
 HCO+H<=>CO+H2 7.340E+013 0.000
 0.0

!REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
 HCO+O<=>CO+OH 3.020E+013 0.000
 0.0
 HCO+O<=>CO2+H 3.000E+013 0.000
 0.0

!REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

HCO+OH<=>CO+H2O 0.0	3.011E+013	0.000
!REF:TIMONEN ET AL., JPC, 92:651 (1988)		
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) HCO+HO2=>CO2+H+OH 0.0	3.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) HCO+HCO=>H2+CO+CO 0.0	3.000E+012	0.000
!REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987) HCO+CH3<=>CH4+CO 0.0	2.650E+013	0.000
!REF:N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005) CH2O+O2<=>HCO+HO2 53420.0	8.070E+015	0.000
!REF: HCO+O2<=>O2CHO -1100.0	1.200E+011	0.000
!REF:ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986 CH2O+O2CHO<=>HCO+HO2CHO 11660.0	1.990E+012	0.000
!REF:WKM ESTIMATE OCHO+OH<=>HO2CHO 0.0	2.000E+013	0.000
!REF: H+CO2<=>OCHO 29000.0	7.500E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) HCO+HCO<=>CH2O+CO 0.0	1.800E+013	0.000
!REF:OH* KATHROTIA ET AL. COMB & FLAME 2010 H+O+M<=>M+OH* 5975.0 H2/ 1.00/ H2O/ 6.50/ O2/ 0.40/ N2/ 0.40/ AR/ 0.35/ OH*+H2O<=>OH+H2O -860.0 OH*+H2<=>OH+H2 -444.0 OH*+N2<=>OH+N2 -1242.0 OH*+OH<=>OH+OH -764.0 OH*+H<=>OH+H -167.0 OH*+AR<=>OH+AR 4135.0	1.500E+013	0.000
	5.930E+012	0.500
	2.950E+012	0.500
	1.080E+011	0.500
	6.010E+012	0.500
	1.310E+012	0.500
	1.690E+012	0.000

OH* \rightleftharpoons OH	1.450E+006	0.000
0.0		
OH*+O2 \rightleftharpoons OH+O2	2.100E+012	0.500
-478.0		
OH*+CO2 \rightleftharpoons OH+CO2	2.750E+012	0.500
-968.0		
OH*+CO \rightleftharpoons OH+CO	3.230E+012	0.500
-787.0		
OH*+CH4 \rightleftharpoons OH+CH4	3.360E+012	0.500
-635.0		
CH+O2 \rightleftharpoons CO+OH*	4.040E+013	0.000
0.0		
C2H+O \rightleftharpoons CO+CH*	6.200E+012	0.000
0.0		
C+H+M \rightleftharpoons CH*+M	6.000E+014	0.000
6940.0		

!REF:DEVRIENDT, VAN LOOK, CEURSTERS, AND PEETERS, CHEM PHYS LETT. 261 (1996) 450, C2H+O2

C2H+O2 \rightleftharpoons CO2+CH*	2.170E+010	0.000
0.0		

!REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

CH*+M \rightleftharpoons CH+M		
CH*+AR \rightleftharpoons CH+AR	4.000E+011	0.500
0.0		
CH*+H2O \rightleftharpoons CH+H2O	5.300E+013	0.000
0.0		
CH*+CO \rightleftharpoons CH+CO	2.440E+012	0.500
0.0		
CH*+CO2 \rightleftharpoons CH+CO2	2.410E-001	4.300
-1694.0		
CH*+O2 \rightleftharpoons CH+O2	2.480E+006	2.140
-1720.0		
CH*+H2 \rightleftharpoons CH+H2	1.470E+014	0.000
1361.0		
CH*+CH4 \rightleftharpoons CH+CH4	1.730E+013	0.000
167.0		
CH* \rightleftharpoons CH	1.860E+006	0.000
0.0		
CH*+N2 \rightleftharpoons CH+N2	3.030E+002	3.400
-381.0		

!REF:LASKIN ET AL. IJCK 32 589-614 2000

HCO+H (+M) \rightleftharpoons CH2O (+M)	1.090E+012	0.480
-260.0		
LOW/	1.350E+024	-2.570
1425.0/		
TROE/ 7.824E-001 2.710E+002 2.755E+003 6.570E+003/		
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/		
3.00/ HE/ 0.70/		
CO+H2 (+M) \rightleftharpoons CH2O (+M)	4.300E+007	1.500
79600.0		
LOW/	5.070E+027	-3.420
84348.0/		
TROE/ 9.320E-001 1.970E+002 1.540E+003 1.030E+004/		
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/		
3.00/ HE/ 0.70/		

!REF:V. VASUDEVAN ET AL. IJCK. 37: 98--109 (2005). CH2O+OH<=>HCO+H2O -1055.0	7.820E+007	1.630
!REF:IRDAM ET AL., IJCK 1993, 25, 285 CH2O+H<=>HCO+H2 2740.0	5.740E+007	1.900
!REF:CURRAN FIT TO NIST DATABASE CH2O+O<=>HCO+OH 2260.0	6.260E+009	1.150
!REF:BAULCH ET AL.		
!REF:JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA:		
!REF:34, 3, 757-1397 2005 CH2O+CH3<=>HCO+CH4 4312.0	3.830E+001	3.360
!REF:J. PHYS. CHEM. A 109, 12027-12035, 2005 CH2O+HO2<=>HCO+H2O2 11520.0	1.880E+004	2.700
!REF:PHIL TAYLOR CH3CHO+OH X 1.5		
!REF:26TH INTL. COMBUSTION SYMP. P 497--504. CH2O+OH<=>HOCH2O 0.0	4.500E+015	-1.100
!REF:CURRAN ESTIMATE HOCH2O<=>HOCHO+H 14900.0	1.000E+014	0.000
!REF:BLAKE ET AL. J. CHEM. SOC. B: 10, 1923 (1971) HOCHO<=>CO+H2O 60470.0 HOCHO<=>CO2+H2 48520.0	2.450E+012 2.950E+009	0.000 0.000
!REF:CURRAN ESTIMATE OCHO+HO2<=>HOCHO+O2 -3275.0	3.500E+010	0.000
!REF:MARINOV ESTIMATE HOCHO+OH=>H2O+CO2+H 916.0 HOCHO+OH=>H2O+CO+OH -962.0 HOCHO+H=>H2+CO2+H 4868.0	2.620E+006 1.850E+007 4.240E+006	2.060 1.510 2.100
!REF:MARINOV ESTIMATE HOCHO+H=>H2+CO+OH 2988.0 HOCHO+CH3=>CH4+CO+OH 2200.0	6.030E+013 3.900E-007	-0.350 5.800

!REF: CURRAN ESTIMATE OCHO+H2O2<=>HOCHO+HO2 10000.0	2.400E+012	0.000
!REF:MARINOV ESTIMATE HOCHO+HO2=>H2O2+CO+OH 11920.0	1.000E+012	0.000
!REF:MARINOV ESTIMATE HOCHO+O=>CO+OH+OH 2975.0	1.770E+018	-1.900
!REF:CURRAN ESTIMATE CH2O+OCHO<=>HOCHO+HCO 13600.0	5.600E+012	0.000
!REF:HIPPLER ET AL. PCCP. 3: 3450--2458 (2001). CH3O(+M)<=>CH2O+H(+M) 26170.0 LOW/ 24307.0/ TROE/ 9.000E-001 2.500E+003 1.300E+003 1.000E+099/ H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/	6.800E+013 1.867E+025	0.000 -3.000
!REF:WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653 (1987) CH3O+O2<=>CH2O+HO2 -5501.0	4.380E-019	9.500
!REF:FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998). CH2O+CH3O<=>CH3OH+HCO 2294.0	6.620E+011	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) CH3+CH3OH<=>CH4+CH3O 6935.0	1.440E+001	3.100
!REF: CH3O+CH3<=>CH2O+CH4 0.0	1.200E+013	0.000
!REF:HOYERMANN ET AL., 18TH SYMPOSIUM CH3O+H<=>CH2O+H2 0.0	2.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) CH3O+HO2<=>CH2O+H2O2 0.0	3.010E+011	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 CH2O+H(+M)<=>CH2OH(+M) 3600.0 LOW/ 6530.0/ TROE/ 7.187E-001 1.030E+002 1.291E+003 4.160E+003/ H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/	5.400E+011 1.270E+032	0.454 -4.820
!REF:GROTHER, H. H. ET AL., J. PHYS. CHEM. 92: 4028 (1988).		

CH2OH+O2<=>CH2O+HO2 0.0 DUP	1.510E+015	-1.000
CH2OH+O2<=>CH2O+HO2 5017.0 DUP	2.410E+014	0.000
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH2OH+H<=>CH2O+H2 0.0	6.000E+012	0.000
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+HO2<=>CH2O+H2O2 0.0	1.200E+013	0.000
!REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998)		
CH2OH+HCO<=>CH2O+CH2O 0.0	1.800E+014	0.000
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+CH3O<=>CH2O+CH3OH 0.0	2.400E+013	0.000
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+HCO<=>CH2OH+CH2O 13110.0	9.630E+003	2.900
OH+CH2OH<=>H2O+CH2O 0.0	2.400E+013	0.000
O+CH2OH<=>OH+CH2O 0.0	4.200E+013	0.000
CH2OH+CH2OH<=>CH2O+CH3OH 0.0	3.000E+012	0.000
!REF:CURRAN ESTIMATE		
CH2OH+HO2<=>HOCH2O+OH 0.0	1.000E+013	0.000
CH2O+HO2<=>OCH2O2H 11900.0	1.500E+011	0.000
OCH2O2H<=>HOCH2O2 8600.0	3.000E+011	0.000
HOCH2O2+HO2<=>HOCH2O2H+O2 -3275.0	3.500E+010	0.000
HOCH2O+OH<=>HOCH2O2H 0.0	1.000E+013	0.000
!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950		
!REF:NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT		
CH3OH (+M) <=> CH3+OH (+M) 92540.6	2.084E+018	-0.615
LOW/ 97992.2/	1.500E+043	-6.995
TROE/ -4.748E-001 3.558E+004 1.116E+003 9.023E+003/		
CH3OH (+M) <=> CH2 (S) + H2O (+M) 91712.0	3.121E+018	-1.017
LOW/ 99417.1/	1.430E+047	-8.227
TROE/ 2.545E+000 3.290E+003 4.732E+004 4.711E+004/		

CH3OH (+M) <=> CH2OH+H (+M)	7.896E-003	5.038
84467.4		
LOW/	3.390E+042	-7.244
105230.3/		
TROE/ -7.391E+001 3.705E+004 4.150E+004 5.220E+003/		
!REF:J. CHEM. PHYS. 134, 094302 (2011)		
CH3OH+H<=>CH2OH+H2	3.070E+005	2.550
5440.0		
CH3OH+H<=>CH3O+H2	1.990E+005	2.560
10300.0		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+O<=>CH2OH+OH	3.880E+005	2.500
3080.0		
!REF:XU ET AL. PROC 31 2007 159-166		
CH3OH+OH<=>CH2OH+H2O	3.080E+004	2.650
-806.7		
CH3OH+OH<=>CH3O+H2O	1.500E+002	3.030
-763.0		
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
CH3OH+O2<=>CH2OH+HO2	2.050E+013	0.000
44900.0		
!REF:CURRAN ESTIMATE		
CH3OH+HO2<=>CH2OH+H2O2	1.080E+004	2.550
10530.0		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+CH3<=>CH2OH+CH4	3.190E+001	3.170
7172.0		
CH3O+CH3OH<=>CH2OH+CH3OH	3.000E+011	0.000
4074.0		
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3O+CH3O<=>CH3OH+CH2O	6.030E+013	0.000
0.0		
!REF:GRI		
CH3+H (+M) <=> CH4 (+M)	1.270E+016	-0.630
383.0		
LOW/	2.477E+033	-4.760
2440.0/		
TROE/ 7.830E-001 7.400E+001 2.941E+003 6.964E+003/		
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/		
3.00/ HE/ 0.70/		
!REF:BAULCH, D.L.; ET AL., J. PHYS. CHEM. REF. DATA (2005)		
CH4+H<=>CH3+H2	6.140E+005	2.500
9587.0		
!REF:CURRAN, FIT TO NIST DATABASE		
CH4+OH<=>CH3+H2O	5.830E+004	2.600
2190.0		

!REF:GRI 3.0
CH4+O<=>CH3+OH 1.020E+009 1.500
8600.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.

!REF:X1.5
CH4+HO2<=>CH3+H2O2 1.695E+001 3.740
21010.0

!REF:GRI 3.0
CH4+CH2<=>CH3+CH3 2.460E+006 2.000
8270.0

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950

!REF:ONLY INCLUDING TRANS HCOH FOR SIMPLICITY, DO NOT HAVE TO COMBINE THE K'S.

!REF:IT'S NOT REALLY SIGNIFICANT ANYWAY
CH3+OH<=>CH2(S)+H2O 4.936E+014 -0.669
-445.8
PLOG/ 0.0100 4.936E+014 -0.669 -445.8/
PLOG/ 0.1000 1.207E+015 -0.778 -175.6/
PLOG/ 1.0000 5.282E+017 -1.518 1772.0/
PLOG/ 10.0000 4.788E+023 -3.155 7003.0/
PLOG/ 100.0000 8.433E+019 -1.962 8244.0/

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950
CH3+OH<=>CH2O+H2 3.502E+005 1.441
-3244.0
PLOG/ 0.0100 3.502E+005 1.441 -3244.0/
PLOG/ 0.1000 8.854E+005 1.327 -2975.0/
PLOG/ 1.0000 1.650E+007 0.973 -2010.0/
PLOG/ 10.0000 5.374E+009 0.287 280.0/
PLOG/ 100.0000 9.494E+018 -2.199 9769.0/

!REF:INCREASED BY FACTOR OF 2 TO IMPROVE AGREEMENT WITH CH4 FLAMESPEED
CH3+OH<=>CH2OH+H 1.621E+010 0.965
3210.0
PLOG/ 0.0100 1.621E+010 0.965 3214.0/
PLOG/ 0.1000 1.807E+010 0.950 3247.0/
PLOG/ 1.0000 4.686E+010 0.833 3566.0/
PLOG/ 10.0000 1.525E+013 0.134 5641.0/
PLOG/ 100.0000 3.590E+014 -0.186 8601.0/

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950
CH3+OH<=>H+CH3O 1.186E+009 1.016
11940.0
PLOG/ 0.0100 1.186E+009 1.016 11940.0/
PLOG/ 0.1000 1.188E+009 1.016 11940.0/
PLOG/ 1.0000 1.230E+009 1.011 11950.0/
PLOG/ 10.0000 1.798E+009 0.965 12060.0/
PLOG/ 100.0000 5.242E+010 0.551 13070.0/
CH3+OH<=>HCOH+H2 8.674E+008 0.787
-3046.0
PLOG/ 0.0100 8.674E+008 0.787 -3046.0/

PLOG/	0.1000	3.115E+009	0.630	-2669.0/	
PLOG/	1.0000	1.557E+011	0.156	-1368.0/	
PLOG/	10.0000	1.704E+021	-2.641	6412.0/	
PLOG/	100.0000	7.250E+020	-2.402	9639.0/	
CH3+OH<=>CH2+H2O				4.293E+004	2.568
3997.8					
!REF:MARINOV 1996					
HCOH+OH<=>HCO+H2O				2.000E+013	0.000
0.0					
HCOH+H<=>CH2O+H				2.000E+014	0.000
0.0					
HCOH+O=>CO2+H+H				5.000E+013	0.000
0.0					
HCOH+O=>CO+OH+H				3.000E+013	0.000
0.0					
HCOH+O2=>CO2+H+OH				5.000E+012	0.000
0.0					
HCOH+O2<=>CO2+H2O				3.000E+013	0.000
0.0					
!REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279-286					
CH3+HO2<=>CH3O+OH				1.000E+012	0.269
-687.5					
CH3+HO2<=>CH4+O2				1.160E+005	2.230
-3022.0					
!REF:HARDING AND KLIPPENSTEIN 2B04, 30TH SYMP 2004.					
CH3+O<=>CH2O+H				5.540E+013	0.050
-136.0					
!REF:N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005)					
CH3+O2<=>CH3O+O				7.546E+012	0.000
28320.0					
!REF: PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN					
CH3+O2<=>CH2O+OH				2.641E+000	3.283
8105.0					
!REF:R.X. FERNANDES ET AL., J PHYS. CHEM. A, (2006) 110:4442-4449.					
CH3+O2 (+M) <=> CH3O2 (+M)				7.812E+009	0.900
0.0					
LOW/				6.850E+024	-3.000
0.0/					
TROE/	6.000E-001	1.000E+003	7.000E+001	1.700E+003/	
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)					
CH3O2+CH2O<=>CH3O2H+HCO				1.990E+012	0.000
11660.0					
!REF:NEW FIT FROM HJC					
!REF:X1.5					
CH4+CH3O2<=>CH3+CH3O2H				9.600E-001	3.770
17810.0					
!REF:TSANG, JPC REF. DATA, 16:471 (1987)					

CH3OH+CH3O2<=>CH2OH+CH3O2H 13710.0	1.810E+012	0.000
!REF:KEIFFER, M. ET AL., J. CHEM. SOC. FARADAY TRANS. 2: 84, 505 (1988)		
CH3O2+CH3<=>CH3O+CH3O -1411.0	5.080E+012	0.000
!REF: LIGHTFOOT, P.D. ETAL., ATMOS. ENVIRON. PART A: 26, 1805-1961 (1992)		
CH3O2+HO2<=>CH3O2H+O2 -1570.0	2.470E+011	0.000
!REF: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220.		
CH3O2+CH3O2=>CH2O+CH3OH+O2 -1051.0	3.110E+014	-1.610
CH3O2+CH3O2=>O2+CH3O+CH3O 1860.0	1.400E+016	-1.610
CH3O2+H<=>CH3O+OH 0.0	9.600E+013	0.000
CH3O2+O<=>CH3O+O2 0.0	3.600E+013	0.000
CH3O2+OH<=>CH3OH+O2 0.0	6.000E+013	0.000
CH3O2H<=>CH3O+OH 42300.0	6.310E+014	0.000
!REF:GRI		
CH2 (S) +N2<=>CH2+N2 600.0	1.500E+013	0.000
CH2 (S) +AR<=>CH2+AR 600.0	9.000E+012	0.000
CH2 (S) +H<=>CH+H2 0.0	3.000E+013	0.000
CH2 (S) +O<=>CO+H2 0.0	1.500E+013	0.000
CH2 (S) +O<=>HCO+H 0.0	1.500E+013	0.000
CH2 (S) +OH<=>CH2O+H 0.0	3.000E+013	0.000
CH2 (S) +H2<=>CH3+H 0.0	7.000E+013	0.000
CH2 (S) +O2=>H+OH+CO 0.0	2.800E+013	0.000
CH2 (S) +O2<=>CO+H2O 0.0	1.200E+013	0.000
CH2 (S) +H2O<=>CH2+H2O 0.0	3.000E+013	0.000
CH2 (S) +CO<=>CH2+CO 0.0	9.000E+012	0.000
CH2 (S) +CO2<=>CH2+CO2 0.0	7.000E+012	0.000
CH2 (S) +CO2<=>CH2O+CO 0.0	1.400E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
CH2+H (+M) <=>CH3 (+M) 0.0	2.500E+016	-0.800
LOW/ 1230.0/	3.200E+027	-3.140

TROE/ 6.800E-001 7.800E+001 1.995E+003 5.590E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/

!REF:GRI 3.0

CH2+O2<=>HCO+OH	1.060E+013	0.000
1500.0		
CH2+O2=>CO2+H+H	2.640E+012	0.000
1500.0		
CH2+O=>CO+H+H	5.000E+013	0.000
0.0		
CH2+OH<=>CH+H2O	1.130E+007	2.000
3000.0		
CH+O2<=>HCO+O	3.300E+013	0.000
0.0		

!REF:GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO
(1985)

C+OH<=>CO+H	5.000E+013	0.000
0.0		
C+O2<=>CO+O	5.000E+013	0.000
0.0		

!REF: GRI

CH+H<=>C+H2	1.100E+014	0.000
0.0		

!REF:MESSING ET AL., J. CHEM. PHYS. 74, 3874 (1981)

CH+O<=>CO+H	5.700E+013	0.000
0.0		

!REF:GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO
(1985)

CH+OH<=>HCO+H	3.000E+013	0.000
0.0		
CH2+H<=>CH+H2	3.000E+013	0.000
0.0		

!REF:MAYER, S. W. ET AL., ELEVENTH INTERNATIONAL SYMPOSIUM ON COMBUSTION

!REF:BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21 (2009)

CH+H2O<=>H+CH2O	1.774E+016	-1.220
23.8		

!REF:SMITH ET AL., GRI MECH VERSION 2.11

!REF:1/ 2 OF BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73,
1982

CH+CO2<=>HCO+CO	1.700E+012	0.000
685.0		

!REF:WANG ET AL., JPC A 107:11414 (2003)

CH3+CH3 (+M) <=> C2H6 (+M)	2.277E+015	-0.690
174.9		
LOW/	8.054E+031	-3.750
981.6/		

TROE/ 0.000E+000 5.700E+002 1.000E+030 1.000E+030/
H2O/ 5.00/ CO/ 2.00/ CO2/ 3.00/

!REF:GRI 3.0
 C2H5+H (+M) <=>C2H6 (+M) 5.210E+017 -0.990
 1580.0
 LOW/ 1.990E+041 -7.080
 6685.0/
 TROE/ 8.420E-001 1.250E+002 2.219E+003 6.882E+003/
 H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
 3.00/ HE/ 0.70/
 C2H6+H<=>C2H5+H2 1.150E+008 1.900
 7530.0

!REF: *MIYOSHI, A. ET AL., CHEM. PHYS. LETT. 204, 241-247 (1993)
 C2H6+O<=>C2H5+OH 3.550E+006 2.400
 5830.0

!REF:CURRAN, FIT TO NIST DATABASE
 C2H6+OH<=>C2H5+H2O 1.480E+007 1.900
 950.0

!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)
 C2H6+O2<=>C2H5+HO2 6.030E+013 0.000
 51870.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
 C2H6+CH3<=>C2H5+CH4 5.550E-004 4.720
 3231.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-
 7054.
 C2H6+HO2<=>C2H5+H2O2 3.460E+001 3.610
 16920.0

!REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003
 C2H6+CH3O2<=>C2H5+CH3O2H 1.940E+001 3.640
 17100.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
 C2H6+CH3O<=>C2H5+CH3OH 2.410E+011 0.000
 7090.0
 C2H6+CH<=>C2H5+CH2 1.100E+014 0.000
 -260.0

!REF:MILLER, J.A. AND BOWMAN, C.T.,

!REF:MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN COMBUSTION, WSS/ CI,
 AUTUMN 1988
 CH2 (S)+C2H6<=>CH3+C2H5 1.200E+014 0.000
 0.0

!REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202

!REF:HP AND LP LIMIT*0.7
 C2H4+H (+M) <=>C2H5 (+M) 9.569E+008 1.463
 1355.0
 LOW/ 1.419E+039 -6.642
 5769.0/
 TROE/ -5.690E-001 2.990E+002 -9.147E+003 1.524E+002/

H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/

!REF:

H2+CH3O2<=>H+CH3O2H 1.500E+014 0.000
26030.0

H2+C2H5O2<=>H+C2H5O2H 1.500E+014 0.000
26030.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
C2H4+C2H4<=>C2H5+C2H3 4.820E+014 0.000
71530.0

!REF:ZHU, R.S. ET AL., J. CHEM. PHYS. 120:6566:6573 (2004)
CH3+C2H5<=>CH4+C2H4 1.180E+004 2.450
-2921.0

!REF:STEWART ET AL C&F 1989
CH3+CH3<=>H+C2H5 4.740E+012 0.105
10664.3

PLOG/ 0.0100 4.740E+012 0.105 10664.3/

PLOG/ 0.1000 2.570E+013 -0.096 11406.1/

PLOG/ 1.0000 3.100E+014 -0.362 13372.5/

PLOG/ 10.0000 2.150E+010 0.885 13532.5/

PLOG/ 100.0000 1.032E+002 3.230 11236.1/

!REF:CURRAN: FIT TO PRATT/ WOOD 84 AND PRATT/ VELDMAN 76
C2H5+H<=>C2H4+H2 2.000E+012 0.000
0.0

!REF:GRI 3.0
C2H5+O<=>CH3CHO+H 1.100E+014 0.000
0.0

!REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS
C2H5+HO2<=>C2H5O+OH 1.100E+013 0.000
0.0

!REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS
CH3O2+C2H5<=>CH3O+C2H5O 8.000E+012 0.000
-1000.0

!REF: HARTMANN ET AL. 1990
C2H5O+O2<=>CH3CHO+HO2 4.280E+010 0.000
1097.0

!REF: CURRAN ESTIMATE
CH3+CH2O<=>C2H5O 3.000E+011 0.000
6336.0

!REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
CH3CHO+H<=>C2H5O 4.610E+007 1.710
7090.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
C2H5O2+CH2O<=>C2H5O2H+HCO 1.990E+012 0.000
11660.0

!REF:BASED ON CH4+CH3O2					
CH4+C2H5O2<=>CH3+C2H5O2H				1.810E+011	0.000
18480.0					
!REF:TSANG, JPC REF. DATA, 16:471 (1987)					
CH3OH+C2H5O2<=>CH2OH+C2H5O2H				1.810E+012	0.000
13710.0					
C2H5O2+HO2<=>C2H5O2H+O2				1.750E+010	0.000
-3275.0					
!REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003					
C2H6+C2H5O2<=>C2H5+C2H5O2H				8.600E+000	3.760
17200.0					
C2H5O2H<=>C2H5O+OH				6.310E+014	0.000
42300.0					
C2H5+O2<=>C2H5O2				3.398E+053	-13.900
9279.0					
PLOG/	0.0400	3.398E+053	-13.900	9279.0/	
PLOG/	1.0000	9.362E+059	-15.280	14240.0/	
PLOG/	10.0000	1.262E+060	-14.910	16240.0/	
C2H5+O2<=>C2H4O2H				2.103E+034	-9.010
5444.0					
PLOG/	0.0400	2.103E+034	-9.010	5444.0/	
PLOG/	1.0000	4.884E+033	-8.310	7710.0/	
PLOG/	10.0000	1.705E+045	-11.490	14590.0/	
C2H5+O2<=>C2H4+HO2				2.094E+009	0.490
-391.4					
DUP					
PLOG/	0.0400	2.094E+009	0.490	-391.4/	
PLOG/	1.0000	1.843E+007	1.130	-720.6/	
PLOG/	10.0000	7.561E+014	-1.010	4749.0/	
C2H5+O2<=>C2H4+HO2				6.609E+000	3.510
14160.0					
DUP					
C2H5+O2<=>C2H4O1-2+OH				1.303E+003	1.930
-502.7					
PLOG/	0.0400	1.303E+003	1.930	-502.7/	
PLOG/	1.0000	2.438E+002	2.180	-62.5/	
PLOG/	10.0000	4.621E+009	0.150	5409.0/	
C2H5+O2<=>CH3CHO+OH				4.908E-006	4.760
254.3					
PLOG/	0.0400	4.908E-006	4.760	254.3/	
PLOG/	1.0000	6.803E-002	3.570	2643.0/	
PLOG/	10.0000	8.265E+002	2.410	5285.0/	
C2H4O2H<=>C2H5O2				2.653E-016	6.960
2396.0					
PLOG/	0.0400	2.653E-016	6.960	2396.0/	
PLOG/	1.0000	1.064E+041	-10.100	26030.0/	
PLOG/	10.0000	1.203E+036	-8.130	27020.0/	
C2H5O2<=>CH3CHO+OH				1.237E+035	-9.420
36360.0					
PLOG/	0.0400	1.237E+035	-9.420	36360.0/	
PLOG/	1.0000	1.687E+036	-9.220	38700.0/	
PLOG/	10.0000	2.520E+041	-10.200	43710.0/	
C2H5O2<=>C2H4+HO2				1.782E+032	-7.100
32840.0					
PLOG/	0.0400	1.782E+032	-7.100	32840.0/	
PLOG/	1.0000	2.701E+037	-8.470	35840.0/	

PLOG/	10.0000	1.980E+038	-8.460	37900.0/	
C2H5O2<=>C2H4O1-2+OH				5.778E+045	-11.900
4112.0					
PLOG/	0.0400	5.778E+045	-11.900	4112.0/	
PLOG/	1.0000	1.916E+043	-10.750	42400.0/	
PLOG/	10.0000	3.965E+043	-10.460	45580.0/	
C2H4O2H<=>C2H4O1-2+OH				8.959E+038	-9.400
20660.0					
PLOG/	0.0400	8.959E+038	-9.400	20660.0/	
PLOG/	1.0000	1.224E+037	-8.320	21460.0/	
PLOG/	10.0000	8.848E+030	-6.080	20660.0/	
C2H4O2H<=>C2H4+HO2				3.918E+040	-10.200
22250.0					
PLOG/	0.0400	3.918E+040	-10.200	22250.0/	
PLOG/	1.0000	6.825E+040	-9.610	23840.0/	
PLOG/	10.0000	3.980E+034	-7.250	23250.0/	
C2H4O2H<=>CH3CHO+OH				5.819E+026	-7.970
20860.0					
PLOG/	0.0400	5.819E+026	-7.970	20860.0/	
PLOG/	1.0000	5.520E+034	-9.880	26230.0/	
PLOG/	10.0000	1.188E+034	-9.020	29210.0/	
!REF:LIFSHITZ ET AL. 1983					
C2H4O1-2<=>CH3+HCO				3.630E+013	0.000
57200.0					
!REF:CURRAN, FIT TO NIST DATABASE					
C2H4O1-2<=>CH3CHO				7.407E+012	0.000
53800.0					
!REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984)					
C2H4O1-2+OH<=>C2H3O1-2+H2O				1.780E+013	0.000
3610.0					
C2H4O1-2+H<=>C2H3O1-2+H2				8.000E+013	0.000
9680.0					
!REF:ANALOGY WITH ETHENE					
C2H4O1-2+HO2<=>C2H3O1-2+H2O2				1.130E+013	0.000
30430.0					
C2H4O1-2+CH3O2<=>C2H3O1-2+CH3O2H				1.130E+013	0.000
30430.0					
C2H4O1-2+C2H5O2<=>C2H3O1-2+C2H5O2H				1.130E+013	0.000
30430.0					
!REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984)					
C2H4O1-2+CH3<=>C2H3O1-2+CH4				1.070E+012	0.000
11830.0					
C2H4O1-2+CH3O<=>C2H3O1-2+CH3OH				1.200E+011	0.000
6750.0					
C2H3O1-2<=>CH3CO				8.500E+014	0.000
14000.0					
C2H3O1-2<=>CH2CHO				1.000E+014	0.000
14000.0					
!REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO. 2, 2010					
CH3CHO (+M) <=>CH3+HCO (+M)				2.450E+022	-1.740
86355.0					

LOW/ 95912.5/ TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/ CH3CHO (+M) <=> CH4+CO (+M) 86355.0	1.030E+059	-11.300
LOW/ 95912.5/ TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/	1.144E+058	-11.300
!REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010		
CH3CHO+H<=>CH3CO+H2 1220.0	1.310E+005	2.580
CH3CHO+H<=>CH2CHO+H2 5210.0	2.720E+003	3.100
!REF:CURRAN, FIT TO NIST DATABASE		
CH3CHO+O<=>CH3CO+OH 1868.0	5.940E+012	0.000
!REF:JUAN LI'S PHD THESIS		
CH3CHO+OH<=>CH3CO+H2O -619.0	3.370E+012	0.000
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+O2<=>CH3CO+HO2 39150.0	3.010E+013	0.000
!REF: GUPTA ET AL., PROC COMBUST INST 31 (2007) 167-174		
CH3CHO+CH3<=>CH3CO+CH4 1966.0	7.080E-004	4.580
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+HO2<=>CH3CO+H2O2 11920.0	3.010E+012	0.000
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3O2+CH3CHO<=>CH3O2H+CH3CO 11920.0	3.010E+012	0.000
CH3CHO+CH3CO3<=>CH3CO+CH3CO3H 11920.0	3.010E+012	0.000
!REF:TAYLOR ET AL. 1996		
CH3CHO+OH<=>CH3+HOCHO 0.0	3.000E+015	-1.076
CH3CHO+OH<=>CH2CHO+H2O 815.0	1.720E+005	2.400
!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781		
CH3CO (+M) <=> CH3+CO (+M) 16900.0	1.070E+012	0.630
LOW/ 14600.0/ TROE/ 6.290E-001 8.730E+009 5.520E+000 7.600E+007/	5.650E+018	-0.970
!REF:		
CH3CO+H<=>CH2CO+H2 0.0	2.000E+013	0.000

CH3CO+O<=>CH2CO+OH 2.000E+013 0.000
0.0
CH3CO+CH3<=>CH2CO+CH4 5.000E+013 0.000
0.0

!REF:

CH3CO+O2<=>CH3CO3 1.200E+011 0.000
-1100.0
CH3CO3+HO2<=>CH3CO3H+O2 1.750E+010 0.000
-3275.0
H2O2+CH3CO3<=>HO2+CH3CO3H 2.410E+012 0.000
9936.0
CH4+CH3CO3<=>CH3+CH3CO3H 1.810E+011 0.000
18480.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

!REF:ANALOGY TO CH3O2+CH2O

CH2O+CH3CO3<=>HCO+CH3CO3H 1.990E+012 0.000
11660.0

!REF: ANALOGY TO C2H6+HO2

C2H6+CH3CO3<=>C2H5+CH3CO3H 1.700E+013 0.000
20460.0

!REF:SAHETCHIAN ET AL. 1992

CH3CO3H<=>CH3CO2+OH 5.010E+014 0.000
40150.0

!REF:ANALOGY TO CH3CO<=>CH3+CO

CH3CO2+M<=>CH3+CO2+M 4.400E+015 0.000
10500.0

!REF: J. P. SENOSIAIN; S. J. KLIPPENSTEIN; J. A. MILLER, J. PHYS. CHEM. A
110 (17) (2006) 5772-5781.

CH2CHO<=>CH2CO+H 1.430E+15 -0.15
45610.2
PLOG / 1.000E-002 2.39E+25 -4.80 43428.3/
PLOG / 2.500E-002 2.48E+27 -5.23 44308.6/
PLOG / 1.000E-001 2.37E+30 -5.86 46118.9/
PLOG / 1.000E+000 1.32E+34 -6.57 49459.4/
PLOG / 1.000E+001 3.46E+36 -6.92 52984.7/
PLOG / 1.000E+002 1.18E+36 -6.48 55176.6/

!REF: J. P. SENOSIAIN; S. J. KLIPPENSTEIN; J. A. MILLER, J. PHYS. CHEM. A
110 (17) (2006) 5772-5781.

CH2CHO<=>CH3+CO 2.930E+12 0.29
40330.2
PLOG / 1.000E-002 1.16E+30 -6.07 41335.7/
PLOG / 2.500E-002 1.54E+31 -6.27 42482.4/
PLOG / 1.000E-001 6.37E+32 -6.57 44286.7/
PLOG / 1.000E+000 6.51E+34 -6.87 47196.0/
PLOG / 1.000E+001 2.15E+35 -6.76 49552.8/
PLOG / 1.000E+002 2.23E+33 -5.97 50453.0/

!REF: J. P. SENOSIAIN; S. J. KLIPPENSTEIN; J. A. MILLER, J. PHYS. CHEM. A
110 (17) (2006) 5772-5781.

CH3CO<=>CH3+CO				1.070E+12	0.63
16897.2					
PLOG /	1.000E-002	6.88E+14	-1.97	14586.0/	
PLOG /	2.500E-002	2.40E+15	-2.00	14806.6/	
PLOG /	1.000E-001	1.96E+16	-2.09	15198.1/	
PLOG /	1.000E+000	6.45E+18	-2.52	16438.1/	
PLOG /	1.000E+001	8.18E+19	-2.55	17264.8/	
PLOG /	1.000E+002	1.26E+20	-2.32	18014.0/	
!REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791					
CH2CHO+O2<=>O2CH2CHO				1.580E+077	-21.900
19350.0					
PLOG/	0.0100	1.580E+077	-21.900	19350.0/	
PLOG/	0.1000	3.880E+069	-18.840	19240.0/	
PLOG/	1.0000	7.800E+059	-15.400	17650.0/	
PLOG/	10.0000	3.050E+050	-12.200	15630.0/	
CH2CHO+O2<=>CH2CO+HO2				1.880E+005	2.370
23730.0					
PLOG/	0.0100	1.880E+005	2.370	23730.0/	
PLOG/	0.1000	1.880E+005	2.370	27370.0/	
PLOG/	1.0000	2.510E+005	2.330	23800.0/	
PLOG/	10.0000	7.050E+007	1.630	25290.0/	
CH2CHO+O2=>CH2O+CO+OH				2.680E+017	-1.840
6530.0					
PLOG/	0.0100	2.680E+017	-1.840	6530.0/	
PLOG/	0.1000	1.520E+020	-2.580	8980.0/	
PLOG/	1.0000	1.650E+019	-2.220	10340.0/	
PLOG/	10.0000	8.953E+013	-0.600	10120.0/	
CH2CHO+O2<=>HO2CH2CO				3.640E+065	-21.870
19020.0					
PLOG/	0.0100	3.640E+065	-21.870	19020.0/	
PLOG/	0.1000	3.640E+058	-19.000	19090.0/	
PLOG/	1.0000	6.650E+048	-15.550	17460.0/	
PLOG/	10.0000	4.800E+038	-12.140	14960.0/	
O2CH2CHO<=>HO2CH2CO				8.270E+030	-6.650
24500.0					
PLOG/	0.0100	8.270E+030	-6.650	24500.0/	
PLOG/	0.1000	1.730E+026	-4.990	23760.0/	
PLOG/	1.0000	9.030E+019	-2.920	22170.0/	
PLOG/	10.0000	1.430E+016	-1.670	21210.0/	
O2CH2CHO<=>CH2CO+HO2				2.050E+040	-13.310
52150.0					
PLOG/	0.0100	2.050E+040	-13.310	52150.0/	
PLOG/	0.1000	5.720E+045	-14.000	52200.0/	
PLOG/	1.0000	4.160E+055	-15.760	55080.0/	
PLOG/	10.0000	1.120E+061	-16.040	60010.0/	
HO2CH2CO=>CO+CH2O+OH				2.360E+017	-2.950
8100.0					
PLOG/	0.0100	2.360E+017	-2.950	8100.0/	
PLOG/	0.1000	2.380E+018	-2.950	8100.0/	
PLOG/	1.0000	2.510E+019	-2.950	8110.0/	
PLOG/	10.0000	4.160E+020	-3.020	8240.0/	
HO2CH2CO<=>CH2CO+HO2				1.120E+007	-3.760
21680.0					
PLOG/	0.0100	1.120E+007	-3.760	21680.0/	
PLOG/	0.1000	1.100E+008	-3.760	21680.0/	
PLOG/	1.0000	9.200E+008	-3.730	21630.0/	

PLOG/ 10.0000 2.090E+009 -3.550 21220.0/

!REF:LASKIN ET AL. IJCK 32 589-614 2000
 CH2+CO(+M)<=>CH2CO(+M) 8.100E+011 0.000
 0.0
 LOW/ 2.690E+033 -5.110
 7095.0/

TROE/ 5.907E-001 2.750E+002 1.226E+003 5.185E+003/
 H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
 3.00/ HE/ 0.70/

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781

!REF:DEFINED IN THE REVERSE FROM SJK, P DEPENDENCE FROM CHEMDIS

!REF:IMPORTANT FOR ACETONE FLAME SPEEDS
 CH3CO(+M)<=>CH2CO+H(+M) 9.413E+007 1.917
 44987.2
 LOW/ 1.516E+051 -10.270
 55390.0/

TROE/ 6.009E-001 8.103E+009 6.677E+002 5.000E+009/

!!REF:WKM (SEE COMMENTS AT BEGINNING OF FILE 15/ 09/ 2011
 !CH2CO+H<=>HCCO+H2 1.401E+015 -0.171
 8783.2
 !CH2CO+H<=>CH3+CO 7.704E+013 -0.171
 4183.2

!REF: Y. HIDAKA; K. KIMURA; H. KAWANO, COMBUST. FLAME 99 (1) (1994) 18-
 28.
 CH2CO+H<=>HCCO+H2 1.800E+14 0.000
 8600.0

!REF: J. P. SENOSIAIN; S. J. KLIPPENSTEIN; J. A. MILLER, J. PHYS. CHEM. A
 110 (17) (2006) 5772-5781.
 CH2CO+H<=>CH3+CO 7.768E+08 1.45
 2780.1

!REF:CURRAN ESTIMATE
 CH2CO+O<=>CH2+CO2 1.750E+012 0.000
 1350.0

!REF:
 CH2CO+O<=>HCCO+OH 1.000E+013 0.000
 8000.0
 CH2CO+OH<=>HCCO+H2O 1.000E+013 0.000
 2000.0

!REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491.
 CH2CO+OH<=>CH2OH+CO 2.000E+012 0.000
 -1010.0

!REF:WKM CALCULATION, CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
 !CH2CO+CH3<=>C2H5+CO 4.769E+004 2.312
 9468.0
 CH2(S)+CH2CO<=>C2H4+CO 1.600E+014 0.000
 0.0

HCCO+OH=>H2+CO+CO 0.0	1.000E+014	0.000
HCCO+O=>H+CO+CO 0.0	8.000E+013	0.000
!REF: Y. HIDAKA; K. KIMURA; H. KAWANO, COMBUST. FLAME 99 (1) (1994) 18-28.		
!REF: A-FACTOR INCREASED BY TWO.		
CH2CO+CH3<=>C2H5+CO 0.0	1.800E+011	0.000
CH2CO+CH3<=>HCCO+CH4 25833.6	7.500E+012	0.000
!REF:GRI		
HCCO+H<=>CH2(S)+CO 0.0	1.000E+014	0.000
!REF:KLIPPENSTEIN 2002		
HCCO+O2=>OH+CO+CO 1020.0	1.910E+011	-0.020
HCCO+O2=>CO2+CO+H 1150.0	4.780E+012	-0.142
!REF:FULLE, D.; HIPPLER, H.; STRIEBEL, F.		
!REF:J. CHEM. PHYS. 108: 6709-6716 1998		
CH+CO+M<=>HCCO+M 0.0	7.570E+022	-1.900
!REF:REG 2.11		
CH+CH2O<=>H+CH2CO -515.0	9.460E+013	0.000
CH+HCCO<=>CO+C2H2 0.0	5.000E+013	0.000
!REF:GRI 3.0		
C2H3+H(+M)<=>C2H4(+M) 280.0	6.080E+012	0.270
LOW/ 3320.0/ TROE/ 7.820E-001 2.075E+002 2.663E+003 6.095E+003/ H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/	1.400E+030	-3.860
!REF:GRI		
C2H4(+M)<=>H2+H2CC(+M) 88770.0	8.000E+012	0.440
LOW/ 99860.0/ TROE/ 7.345E-001 1.800E+002 1.035E+003 5.417E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/	7.000E+050	-9.310
!REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996)		
C2H4+H<=>C2H3+H2 12950.0	5.070E+007	1.930
!REF:BAULCH ET AL.		

!REF: JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA:

!REF: 34, 3, 757-1397 2005

!REF: MAKING BRANCHING RATIO 55:45

C2H4+O<=>CH3+HCO	7.453E+006	1.880
183.0		
C2H4+O<=>CH2CHO+H	6.098E+006	1.880
183.0		

!REF: J. PHYS. CHEM 109 2005 7489-7499 (PEETERS)

!REF: FROM STANFORD

C2H4+OH<=>C2H3+H2O	2.230E+004	2.745
2215.5		

!REF: SJK, J PHYS CHEM 110 2006 6960-6970

C2H4+OH<=>CH3+CH2O	5.350E+000	2.920	
-1732.7			
PLOG/ 0.0100	5.350E+000	2.920	-1732.7/
PLOG/ 0.0250	3.190E+001	2.710	-1172.3/
PLOG/ 0.1000	5.550E+002	2.360	-180.8/
PLOG/ 1.0000	1.780E+005	1.680	2060.5/
PLOG/ 10.0000	2.370E+009	0.560	6006.7/
PLOG/ 100.0000	2.760E+013	-0.500	11455.1/
C2H4+OH<=>CH3CHO+H	2.370E-007	5.300	
-2050.6			
PLOG/ 0.0100	2.370E-007	5.300	-2050.6/
PLOG/ 0.0250	8.730E-005	4.570	-618.0/
PLOG/ 0.1000	4.030E-001	3.540	1881.7/
PLOG/ 1.0000	2.380E-002	3.910	1722.7/
PLOG/ 10.0000	8.250E+008	1.010	10507.3/
PLOG/ 100.0000	6.800E+009	0.810	13867.3/
C2H4+OH<=>C2H3OH+H	1.040E+004	2.600	
4121.0			
PLOG/ 0.0100	1.040E+004	2.600	4121.0/
PLOG/ 0.0250	1.070E+004	2.600	4129.0/
PLOG/ 0.1000	1.520E+004	2.560	4238.3/
PLOG/ 1.0000	3.190E+005	2.190	5255.6/
PLOG/ 10.0000	1.940E+008	1.430	7828.8/
PLOG/ 100.0000	8.550E+010	0.750	11490.8/
C2H4+OH<=>PC2H4OH	1.740E+043	-10.461	
7698.7			
PLOG/ 0.0100	1.740E+043	-10.461	7698.7/
PLOG/ 0.0250	3.250E+037	-8.629	5214.7/
PLOG/ 0.1000	1.840E+035	-7.750	4908.9/
PLOG/ 1.0000	2.560E+036	-7.752	6946.1/
PLOG/ 10.0000	3.700E+033	-6.573	7605.9/
PLOG/ 100.0000	1.120E+026	-4.101	5757.0/

!REF: ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+O2<=>CH2CHO+HO2	5.310E+011	0.210
39830.0		
C2H3OH+O<=>CH2CHO+OH	1.875E+006	1.900
-860.0		
!C2H3OH+OH<=>CH2CHO+H2O	3.330E+009	1.100
540.5		

C2H3OH+CH3<=>CH2CHO+CH4 2.030E-008 5.900
1052.0
C2H3OH+CH3O2<=>CH2CHO+CH3O2H 3.400E+003 2.500
8922.0

!REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608,

!REF:EXCEPT FOR SC2H4OH CHANNEL KEPT WKM CALCULATION

C2H3OH+H<=>CH2CHO+H2 1.480E+003 3.077
7220.0
C2H3OH+H<=>C2H2OH+H2 2.470E+007 2.030
15200.0
C2H3OH+H<=>PC2H4OH 3.010E+008 1.577
3670.0

!REF:DA SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483 (2009) 25-29

C2H3OH+HO2<=>CH3CHO+HO2 1.490E+005 1.670
6810.0

!REF:JU-XIANG SHAO THEOR CHEM ACC (2011) 128:341-348

!REF:CHANGED PRODUCTS FROM CH3+HCO

C2H3OH<=>CH3CHO 7.420E+046 -10.560
67420.0
PLOG/ 0.1000 7.420E+046 -10.560 67420.0/
PLOG/ 1.0000 4.420E+042 -9.090 67069.2/
PLOG/ 100.0000 2.900E+027 -4.350 61612.9/

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

!REF:WKM 19/ 04/ 2010

!REF:TAKEN FROM SAN DIEGO MECH

!REF: MARINOV, 1995

!REF:CHECK EFFECT!!!!

C2H4+O2<=>C2H3+HO2 4.220E+013 0.000
57623.1

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

C2H4+CH3O<=>C2H3+CH3OH 1.200E+011 0.000
6750.0

!REF:WKM 22/ 04/ 2010

!REF:FROM BILL PITZ'S SUGGESTION

C2H4+CH3O2<=>C2H3+CH3O2H 8.590E+000 3.754
27132.0

!REF:WKM 22/ 04/ 2010

!REF:FROM BILL PITZ'S SUGGESTION

C2H4+C2H5O2<=>C2H3+C2H5O2H 8.590E+000 3.754
27132.0

!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)

C2H4+CH3CO3<=>C2H3+CH3CO3H 30430.0	1.130E+013	0.000
!REF:PITZ ESTIMATE		
C2H4+CH3O2<=>C2H4O1-2+CH3O 17110.0	2.820E+012	0.000
C2H4+C2H5O2<=>C2H4O1-2+C2H5O 17110.0	2.820E+012	0.000
!REF:BAULCH AND COBOS REDUCED BY A FACTOR OF 4		
C2H4+HO2<=>C2H4O1-2+OH 17190.0	5.575E+011	0.000
!REF:BUTLER, FLEMING, GOSS, LIN, ACS SYMP. SER. 134 (1980).		
CH+CH4<=>C2H4+H 0.0	6.000E+013	0.000
!REF:MARINOV ESTIMATE.		
CH2(S)+CH3<=>C2H4+H 0.0	2.000E+013	0.000
!REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202		
C2H2+H(+M)<=>C2H3(+M) 2709.0	1.710E+010	1.266
LOW/ 3780.0/	6.346E+031	-4.664
TROE/ 7.880E-001 -1.020E+004 1.000E-030/ H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/		
!REF:N.M MARINOV ET AL., COMBUST. FLAME 114 (1998) 192-213		
!REF:ADOPTING KLIPPENSTEIN'S PRODUCTS FOR ONE OF THE CHANNELS,		
!REF:TO COMBAT OVER-PRODUCTION OF C2H2 IN ETHYLENE JSR		
C2H3+O2<=>CH2O+HCO 6503.1	1.700E+029	-5.312
C2H3+O2<=>CH2CHO+O 5262.4	7.000E+014	-0.611
C2H3+O2=>H+CO+CH2O 3312.6	5.190E+015	-1.260
!REF:		
CH3+C2H3<=>CH4+C2H2 0.0	3.920E+011	0.000
!REF:BILL SUGGESTED		
C2H3+H<=>C2H2+H2 0.0	1.700E+014	0.000
!REF:USC ESTIMATE		
C2H3+H<=>H2CC+H2 0.0	6.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
C2H3+OH<=>C2H2+H2O 0.0	3.011E+013	0.000

C2H3+C2H3<=>C2H2+C2H4	9.600E+011	0.000
0.0		
!REF: GRI 3.0		
C2H+H (+M) <=>C2H2 (+M)	1.000E+017	0.000
0.0		
LOW/	3.750E+033	-4.800
1900.0/		
TROE/ 6.460E-001 1.320E+002 1.315E+003 5.566E+003/		
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/		
3.00/ HE/ 0.70/		
!REF:GRI		
C2H+O<=>CH+CO	5.000E+013	0.000
0.0		
C2H+OH<=>H+HCCO	2.000E+013	0.000
0.0		
C2H+O2<=>HCO+CO	5.000E+013	0.000
1500.0		
C2H+H2<=>H+C2H2	4.900E+005	2.500
560.0		
!REF:99 LAS/ WAN		
C2H2 (+M) <=>H2CC (+M)	8.000E+014	-0.520
50750.0		
LOW/	2.450E+015	-0.640
49700.0/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/		
2.50/ C2H4/ 2.50/		
!REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706		
C2H2+O<=>CH2+CO	7.395E+008	1.280
2472.0		
C2H2+O<=>HCCO+H	2.958E+009	1.280
2472.0		
C2H2+HO2<=>CH2CO+OH	6.030E+009	0.000
7949.0		
!REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055		
C2H2+OH<=>C2H+H2O	2.632E+006	2.140
17060.0		
C2H2+OH<=>HCCOH+H	2.800E+005	2.280
12420.0		
PLOG/ 0.0100	2.800E+005	2.280
PLOG/ 0.0250	7.467E+005	2.160
PLOG/ 0.1000	1.776E+006	2.040
PLOG/ 1.0000	2.415E+006	2.000
PLOG/ 10.0000	3.210E+006	1.970
PLOG/ 100.0000	7.347E+006	1.890
C2H2+OH<=>CH2CO+H	1.578E+003	2.560
-844.5		
PLOG/ 0.0100	1.578E+003	2.560
PLOG/ 0.0250	1.518E+004	2.280
PLOG/ 0.1000	3.017E+005	1.920
PLOG/ 1.0000	7.528E+006	1.550
PLOG/ 10.0000	5.101E+006	1.650
PLOG/ 100.0000	1.457E+004	2.450

C2H2+OH<=>CH3+CO				4.757E+005	1.680
-329.8					
PLOG/	0.0100	4.757E+005	1.680	-329.8/	
PLOG/	0.0250	4.372E+006	1.400	226.5/	
PLOG/	0.1000	7.648E+007	1.050	1115.0/	
PLOG/	1.0000	1.277E+009	0.730	2579.0/	
PLOG/	10.0000	4.312E+008	0.920	3736.0/	
PLOG/	100.0000	8.250E+005	1.770	4697.0/	
C2H2+OH<=>C2H2OH				3.913E+032	-7.126
5824.0					
PLOG/	0.0100	3.913E+032	-7.126	5824.0/	
PLOG/	0.0250	1.067E+032	-6.847	5508.0/	
PLOG/	0.1000	1.646E+032	-6.717	5822.0/	
PLOG/	1.0000	1.387E+031	-6.087	6348.0/	
PLOG/	10.0000	2.892E+029	-5.288	7055.0/	
PLOG/	100.0000	1.367E+025	-3.754	6543.0/	
!REF:GRI 3.0 AND USC II					
C2H2+HCO<=>C2H3+CO				1.000E+007	2.000
6000.0					
C2H2+CH2<=>C3H3+H				1.200E+013	0.000
6620.0					
C2H2+CH2 (S) <=>C3H3+H				2.000E+013	0.000
0.0					
C2H2+HCCO<=>C3H3+CO				1.000E+011	0.000
3000.0					
H2CC+H<=>C2H2+H				1.000E+014	0.000
0.0					
H2CC+OH<=>CH2CO+H				2.000E+013	0.000
0.0					
H2CC+O2<=>HCO+HCO				1.000E+013	0.000
0.0					
!REF:GRI 2.11					
H+HCCOH<=>H+CH2CO				1.000E+013	0.000
0.0					
!REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010					
C2H5OH<=>C2H4+H2O				3.410E+059	-14.200
83672.6					
PLOG/	0.0010	3.410E+059	-14.200	83672.6/	
PLOG/	0.0100	2.620E+057	-13.300	85262.2/	
PLOG/	0.1000	1.650E+052	-11.500	84745.6/	
PLOG/	1.0000	5.230E+043	-8.900	81506.7/	
PLOG/	10.0000	4.590E+032	-5.600	76062.4/	
PLOG/	100.0000	3.840E+020	-2.060	69465.5/	
C2H5OH<=>CH3+CH2OH				1.200E+054	-12.900
100005.7					
PLOG/	0.0010	1.200E+054	-12.900	100005.7/	
PLOG/	0.0100	5.180E+059	-14.000	99906.4/	
PLOG/	0.1000	1.620E+066	-15.300	105390.5/	
PLOG/	1.0000	5.550E+064	-14.500	106183.0/	
PLOG/	10.0000	1.550E+058	-12.300	105768.0/	
PLOG/	100.0000	1.780E+047	-8.960	101058.8/	
C2H5OH<=>C2H5+OH				8.100E+046	-11.300
111053.4					
PLOG/	0.0010	8.100E+046	-11.300	111053.4/	
PLOG/	0.0100	1.860E+056	-13.500	107238.4/	

PLOG/	0.1000	4.650E+063	-15.000	109622.8/	
PLOG/	1.0000	4.460E+065	-14.900	112345.0/	
PLOG/	10.0000	2.790E+061	-13.400	113080.2/	
PLOG/	100.0000	6.170E+051	-10.300	109940.7/	

C2H5OH+O2<=>PC2H4OH+HO2		2.000E+013		0.000
52800.0				

C2H5OH+O2<=>SC2H4OH+HO2		1.500E+013		0.000
50150.0				

!REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010

C2H5OH+H<=>SC2H4OH+H2		8.790E+004		2.680
2910.0				

C2H5OH+H<=>PC2H4OH+H2		5.310E+004		2.810
7490.0				

C2H5OH+H<=>C2H5O+H2		9.450E+002		3.140
8701.1				

!REF: SMB 04/ 09/ 2013

!REF: BRANCHING RATIO CHANGED FOR THE UNDERPREDICIOTN OF C2H4 IN THE JSR AND FLOW REACTOR

C2H5OH+OH<=>SC2H4OH+H2O		7.520E+004		2.490
-1474.1				

C2H5OH+OH<=>PC2H4OH+H2O		3.760E+003		2.780
-1810.2				

C2H5OH+OH<=>C2H5O+H2O		5.810E-003		4.280
-3560.0				

!REF:ESTIMATED FROM CW ZHOU BUTANOL+OH

!REF: MITTAL 2013 (INCREASED BY 1.75 ZHOU)

C2H5OH+HO2<=>SC2H4OH+H2O2		2.450E-005		5.260
7475.1				

C2H5OH+HO2<=>PC2H4OH+H2O2		3.986E-002		4.300
15333.0				

C2H5OH+HO2<=>C2H5O+H2O2		6.470E-007		5.300
10533.1				

!REF:ANAOLGY WITH C2H5OH+HO2

C2H5OH+CH3O2<=>SC2H4OH+CH3O2H		1.225E-005		5.260
7475.1				

C2H5OH+CH3O2<=>PC2H4OH+CH3O2H		1.995E-002		4.300
15333.0				

C2H5OH+CH3O2<=>C2H5O+CH3O2H		3.236E-007		5.300
10533.1				

!REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703

C2H5OH+O<=>PC2H4OH+OH		9.690E+002		3.230
4658.0				

C2H5OH+O<=>SC2H4OH+OH		1.450E+005		2.470
876.0				

C2H5OH+O<=>C2H5O+OH		1.460E-003		4.730
1727.0				

!REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004

C2H5OH+CH3<=>PC2H4OH+CH4		3.300E+002		3.300
12290.0				

C2H5OH+CH3<=>SC2H4OH+CH4 7634.0	1.993E+001	3.370
C2H5OH+CH3<=>C2H5O+CH4 7721.0	2.035E+000	3.570

!REF:1/ 2 OF C4H10+C2H5

C2H5OH+C2H5<=>PC2H4OH+C2H6 13400.0	5.000E+010	0.000
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!REF:ESTIMATE

C2H5OH+C2H5<=>SC2H4OH+C2H6 10400.0	5.000E+010	0.000
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!REF:CURRAN, FIT TO NIST DATABASE

!REF:WKM CALCULATION.

SC2H4OH<=>CH3CHO+H 45049.0	5.690E+052	-13.380
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PLOG/	0.0010	5.690E+052	-13.380	45049.0/
PLOG/	0.0100	3.290E+056	-14.120	48129.0/
PLOG/	0.1000	8.580E+057	-14.160	50743.0/
PLOG/	1.0000	5.360E+055	-13.150	51886.0/
PLOG/	10.0000	1.660E+048	-10.640	50297.0/
PLOG/	20.0000	8.260E+044	-9.590	49218.0/
PLOG/	50.0000	1.010E+040	-8.060	47439.0/
PLOG/	100.0000	1.100E+036	-6.840	45899.0/

SC2H4OH<=>C2H3OH+H 44323.0	5.400E+046	-11.630
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PLOG/	0.0010	5.400E+046	-11.630	44323.0/
PLOG/	0.0100	1.210E+051	-12.550	47240.0/
PLOG/	0.1000	2.870E+054	-13.150	50702.0/
PLOG/	1.0000	3.790E+053	-12.510	52560.0/
PLOG/	10.0000	6.330E+046	-10.200	51441.0/
PLOG/	20.0000	3.870E+043	-9.170	50440.0/
PLOG/	50.0000	5.080E+038	-7.650	48713.0/
PLOG/	100.0000	5.120E+034	-6.410	47182.0/

SC2H4OH<=>C2H5O 44328.0	5.480E+045	-11.630
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PLOG/	0.0010	5.480E+045	-11.630	44328.0/
PLOG/	0.0100	2.540E+049	-12.370	46445.0/
PLOG/	0.1000	1.650E+054	-13.400	50330.0/
PLOG/	1.0000	1.810E+055	-13.310	53132.0/
PLOG/	10.0000	4.580E+049	-11.320	52714.0/
PLOG/	20.0000	4.110E+046	-10.330	51834.0/
PLOG/	50.0000	6.680E+041	-8.830	50202.0/
PLOG/	100.0000	6.540E+037	-7.580	48697.0/

SC2H4OH<=>PC2H4OH 51019.0	2.650E+036	-8.860
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PLOG/	0.0010	2.650E+036	-8.860	51019.0/
PLOG/	0.0100	3.560E+037	-8.890	51114.0/
PLOG/	0.1000	4.140E+039	-9.190	51912.0/
PLOG/	1.0000	5.820E+044	-10.340	55296.0/
PLOG/	10.0000	4.260E+048	-11.060	59458.0/
PLOG/	20.0000	8.840E+047	-10.740	59901.0/
PLOG/	50.0000	2.230E+045	-9.840	59604.0/
PLOG/	100.0000	1.700E+042	-8.830	58737.0/

!REF:BASED ON C3H6OH+O2 REACTION

O2C2H4OH<=>PC2H4OH+O2 3.900E+016 -1.000
30000.0

!REF:

O2C2H4OH=>OH+CH2O+CH2O 3.125E+009 0.000
18900.0

!REF:DA SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933

SC2H4OH+O2<=>CH3CHO+HO2 5.260E+017 -1.638
869.0

PLOG/ 0.0100 5.260E+017 -1.637 838.0/
PLOG/ 0.1000 5.260E+017 -1.637 838.0/
PLOG/ 1.0000 5.280E+017 -1.638 839.0/
PLOG/ 10.0000 1.540E+018 -1.771 1120.0/
PLOG/ 100.0000 3.780E+020 -2.429 3090.0/

SC2H4OH+O2<=>C2H3OH+HO2 5.512E+003 2.495
-414.0

PLOG/ 0.0100 5.120E+002 2.496 -414.0/
PLOG/ 0.1000 5.330E+002 2.490 -402.0/
PLOG/ 1.0000 7.620E+002 2.446 -296.0/
PLOG/ 10.0000 8.920E+003 2.146 470.0/
PLOG/ 100.0000 4.380E+005 1.699 2330.0/

!!REF: SAXENA ET AL. PROCEEDINGS. 32 123-130 (2009)

!CH3COCH3<=>CH3CO+CH3 2.050E+058 -12.796
100030.1

!PLOG/ 0.0100 2.050E+058 -12.796 100030.1/
!PLOG/ 0.1000 3.300E+051 -10.574 98221.2/
!PLOG/ 1.0000 1.310E+042 -7.657 94660.6/
!PLOG/ 10.0000 2.160E+033 -4.989 90916.5/
!PLOG/ 100.0000 9.400E+028 -3.669 89022.8/

!REF: S. SAXENA; J. H. KIEFER; S. J. KLIPPENSTEIN, PROC. COMBUST. INST.
32 (1) (2009) 123-130.

!MECH_136

!REF: A-FACTOR INCREASED BY 2.

CH3COCH3<=>CH3CO+CH3 8.570E+064 -15.33
101115.0

PLOG / 1.000E-004 8.570E+064 -15.33 101115.0/
PLOG / 1.000E-002 2.610E+060 -13.47 100576.0/
PLOG / 1.000E-001 2.320E+056 -12.04 99948.0/
PLOG / 5.000E-001 1.900E+052 -10.69 98852.0/
PLOG / 1.000E+000 1.520E+050 -10.03 98168.0/
PLOG / 8.000E+000 9.260E+042 -7.78 95415.0/
PLOG / 1.000E+001 1.410E+042 -7.53 95074.0/
PLOG / 1.200E+001 3.030E+041 -7.33 94792.0/
PLOG / 1.250E+001 2.140E+041 -7.29 94728.0/
PLOG / 1.300E+001 1.540E+041 -7.24 94667.0/
PLOG / 1.000E+002 1.450E+034 -5.12 91528.0/

!REF: REVERSE OF ESTIMATE FOR RADICAL-H RECOMBINATION [REF!].

!MECH_136

CH3COCH3<=>CH3COCH2+H 1.620E+046 -10.28
107867.0

PLOG / 1.000E-004 1.620E+046 -10.28 107867.0/
PLOG / 1.000E-002 1.020E+047 -9.94 107379.0/
PLOG / 1.000E-001 1.800E+045 -9.15 106725.0/
PLOG / 5.000E-001 1.040E+043 -8.30 106298.0/

PLOG / 1.000E+000 4.990E+041 -7.84 106017.0/
PLOG / 8.000E+000 1.520E+036 -6.03 104402.0/
PLOG / 1.000E+001 2.870E+035 -5.80 104149.0/
PLOG / 1.200E+001 7.110E+034 -5.61 103931.0/
PLOG / 1.250E+001 5.180E+034 -5.56 103881.0/
PLOG / 1.300E+001 3.820E+034 -5.52 103832.0/
PLOG / 1.000E+002 1.990E+027 -3.28 100885.0/

!REF: ANALOGY WITH CH3+C2H4<=>NC3H7.

!REF: H. J. CURRAN, INT. J. CHEM. KINET. 38 (4) (2006) 250-275.

!REF: REVERSED REACTION.

CH3COCH2<=>CH2CO+CH3 1.091E+12 0.5816
39684.7

!REF: ESTIMATE FOR RADICAL-RADICAL RECOMBINATION [REF!].

!REF: REVERSED REACTION.

C2H5COCH3<=>CH3COCH2+CH3 1.223E+19 -0.7362
83928.4

!REF: W. TSANG; R. F. HAMPSON, J. PHYS. CHEM. REF. DATA 15 (3) (1986)
1087-1279.

!REF: REVERSED REACTION.

C2H5COCH3<=>CH3CO+C2H5 2.321E+22 -1.1048
84359.9

!!REF:ESTIMATE

!CH3COCH3+OH<=>CH3COCH2+H2O 1.250E+005 2.483
445.0

!!REF:CURRAN ESTIMATE

!CH3COCH3+H<=>CH3COCH2+H2 9.800E+005 2.430
5160.0

!!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98

!CH3COCH3+O<=>CH3COCH2+OH 5.130E+011 0.211
4890.0

!!REF:

!CH3COCH3+CH3<=>CH3COCH2+CH4 3.960E+011 0.000
9784.0

!!REF:ESTIMATE

!CH3COCH3+CH3O<=>CH3COCH2+CH3OH 4.340E+011 0.000
6460.0

!!REF:A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN

!CH3COCH3+O2<=>CH3COCH2+HO2 6.030E+013 0.000
48500.0

!REF: A-FACTOR BY ANALOGY WITH C3H8+O2<=>NC3H7+HO2 [REF!] AND EA FROM
DHRXN.

!REF: K. P. SOMERS; J. M. SIMMIE; F. GILLESPIE; C. CONROY; G. BLACK; W.
K. METCALFE; F. BATTIN-LECLERC;

!REF: P. DIRRENBERGER; O. HERBINET; P. A. GLAUDE; P. DAGAUT; C. TOGBÉ; K. YASUNAGA; R. X. FERNANDES; C. LEE;

!REF: R. TRIPATHI; H. J. CURRAN, COMBUST. FLAME 160 (11) (2013) 2291-2318.

CH3COCH3+O2<=>CH3COCH2+HO2 6.000E+013 0.000
46255.0

!REF: P. F. AMBIDGE; J. N. BRADLEY; D. A. WHYTOCK, J. CHEM. SOC., FARADAY TRANS. 1 72 (1976) 1870-1876.

CH3COCH3+O<=>CH3COCH2+OH 4.270E+013 0.000
5988.0

!REF: V. VASUDEVAN; D. F. DAVIDSON; R. K. HANSON, J. PHYS. CHEM. A 109 (15) (2005) 3352-3359.

CH3COCH3+OH<=>CH3COCH2+H2O 2.950E+013 0.000
4564.6

!REF: K. SATO; Y. HIDAKA, COMBUST. FLAME 122 (3) (2000) 291-311.

CH3COCH3+H<=>CH3COCH2+H2 2.300E+007 2.000
5000.0

!REF: A-FACTOR INCREASED BY THREE.

CH3COCH3+CH3<=>CH3COCH2+CH4 2.850E+004 2.500
8400.0

!REF: ANALOGY WITH C3H8+CH3O<=>NC3H7+CH3OH.

!REF: W. TSANG, J. PHYS. CHEM. REF, DATA 17 (2) (1988) 887-951.

CH3COCH3+CH3O<=>CH3COCH2+CH3OH 4.340E+011 0.000
6458.0

!REF: S. KOJIMA, COMBUST. FLAME 99 (1) (1994) 87-136.

!REF: REVERSED REACTION.

CH3COCH3+HCO<=>CH3COCH2+CH2O 2.965E+11 0.2526
15303.3

!REF: ANALOGY WITH C3H8+HO2<=>NC3H7+H2O2.

!REF: J. AGUILERA-IPARRAGUIRRE; H. J. CURRAN; W. KLOPPER; J. M. SIMMIE, J. PHYS. CHEM. A 112 (30) (2008) 7047-7054.

CH3COCH3+HO2<=>CH3COCH2+H2O2 4.080E+001 3.590
17160.0

!REF: ANALOGY WITH C3H8+CH3O2<=>NC3H7+CH3O2H.

!REF: J. AGUILERA-IPARRAGUIRRE; H. J. CURRAN; W. KLOPPER; J. M. SIMMIE, J. PHYS. CHEM. A 112 (30) (2008) 7047-7054.

!REF: H.-H. CARSTENSEN; A. M. DEAN; O. DEUTSCHMANN, PROC. COMBUST. INST. 31 (1) (2007) 149-157.

CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H 1.280E+000 3.960
18500.0

!REF: ANALOGY WITH NC3H7+O2<=>NC3H7O2.

!REF: C. FRANKLIN GOLDSMITH; W. H. GREEN; S. J. KLIPPENSTEIN, J. PHYS. CHEM. A 116 (13) (2012) 3325-3346.

CH3COCH2+O2<=>CH3COCH2O2 9.20E+08 0.405
-4398.65

PLOG / 1.000E-002 9.20E+08 0.405 -4398.65/

PLOG / 1.000E-001 1.45E+14 -0.984 -1710.80/

PLOG / 1.000E+000 2.09E+13 -0.499 -938.423/

PLOG / 1.000E+001 1.15E+20 -2.420 2451.26/

PLOG / 1.000E+002 2.07E+16 -1.300 803.419/

!REF: ANALOGY WITH NC3H7+HO2<=>NC3H7O2H.

!REF: C. FRANKLIN GOLDSMITH; S. J. KLIPPENSTEIN; W. H. GREEN, PROC. COMBUST. INST. 33 (1) (2011) 273-282.

CH3COCH2+HO2<=>C3KET21 7.220E+022 -4.66 -
3635.0

PLOG / 1.000E-002 7.220E+022 -4.66 -3635.0/
PLOG / 1.000E-001 2.320E+025 -5.08 -2412.0/
PLOG / 1.000E+000 8.390E+030 -6.32 1737.0/
PLOG / 2.500E+000 1.390E+033 -6.81 3852.0/
PLOG / 8.000E+000 3.840E+034 -7.02 6027.0/
PLOG / 1.000E+001 4.040E+034 -6.99 6320.0/
PLOG / 1.200E+001 3.600E+034 -6.94 6523.0/
PLOG / 1.250E+001 3.440E+034 -6.93 6564.0/
PLOG / 1.000E+002 4.840E+029 -5.22 6327.0/

!REF: ANALOGY WITH NC3H7+HO2<=>NC3H7O+OH.

!REF: C. FRANKLIN GOLDSMITH; S. J. KLIPPENSTEIN; W. H. GREEN, PROC. COMBUST. INST. 33 (1) (2011) 273-282.

CH3COCH2+HO2<=>CH3COCH2O+OH 1.310E+014 -0.43
144.0

PLOG / 1.000E-002 1.310E+014 -0.43 144.0/
PLOG / 1.000E-001 1.360E+015 -0.71 916.0/
PLOG / 1.000E+000 2.840E+019 -1.91 4366.0/
PLOG / 2.500E+000 1.640E+022 -2.67 6750.0/
PLOG / 8.000E+000 4.510E+025 -3.60 10116.0/
PLOG / 1.000E+001 1.590E+026 -3.75 10739.0/
PLOG / 1.200E+001 4.020E+026 -3.85 11231.0/
PLOG / 1.250E+001 4.880E+026 -3.87 11339.0/
PLOG / 1.000E+002 9.270E+026 -3.85 14767.0/

!REF: ANALOGY WITH NC3H7+CH3O2<=>NC3H7O+CH3O.

!REF: C. FRANKLIN GOLDSMITH; S. J. KLIPPENSTEIN; W. H. GREEN, PROC. COMBUST. INST. 33 (1) (2011) 273-282.

CH3COCH2+CH3O2<=>CH3COCH2O+CH3O 1.310E+014 -0.43
144.0

PLOG / 1.000E-002 1.310E+014 -0.43 144.0/
PLOG / 1.000E-001 1.360E+015 -0.71 916.0/
PLOG / 1.000E+000 2.840E+019 -1.91 4366.0/
PLOG / 2.500E+000 1.640E+022 -2.67 6750.0/
PLOG / 8.000E+000 4.510E+025 -3.60 10116.0/
PLOG / 1.000E+001 1.590E+026 -3.75 10739.0/
PLOG / 1.200E+001 4.020E+026 -3.85 11231.0/
PLOG / 1.250E+001 4.880E+026 -3.87 11339.0/
PLOG / 1.000E+002 9.270E+026 -3.85 14767.0/

!REF: ANALOGY WITH NC3H7O2H<=>NC3H7O+OH.

!REF: C. FRANKLIN GOLDSMITH; S. J. KLIPPENSTEIN; W. H. GREEN, PROC. COMBUST. INST. 33 (1) (2011) 273-282.

C3KET21<=>CH3COCH2O+OH 1.250E+051 -11.85
48834.0

PLOG / 1.000E-002 1.250E+051 -11.85 48834.0/
PLOG / 1.000E-001 8.960E+050 -11.43 51438.0/
PLOG / 1.000E+000 2.390E+046 -9.75 51712.0/
PLOG / 2.500E+000 1.200E+043 -8.67 50925.0/
PLOG / 8.000E+000 7.260E+037 -7.02 49220.0/

PLOG / 1.000E+001 5.760E+036 -6.67 48817.0/
PLOG / 1.200E+001 6.990E+035 -6.39 48473.0/
PLOG / 1.250E+001 4.340E+035 -6.32 48395.0/
PLOG / 1.000E+002 1.040E+025 -3.08 43994.0/

!REF: WESTBROOK ESTIMATE [REF!]

!REF: WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
SEATTLE, AUGUST, 1988

CH3COCH2O2+CH3COCH3<=>C3KET21+CH3COCH2
16000.0 2.800E+012 0.000
CH3COCH2O2+CH2O<=>C3KET21+HCO
9000.0 ! ARAMCOMECH 1.3 1.288E+011 0.000
CH3COCH2O2+HO2<=>C3KET21+O2
0.0 ! ARAMCOMECH 1.3 1.000E+012 0.000

!REF: A. M. EL-NAHAS; J. M. SIMMIE; M. V. NAVARRO; J. W. BOZZELLI; G.
BLACK; H. J. CURRAN, PHYS. CHEM. CHEM. PHYS. 10 (47) (2008) 7139-7149.

CH3COCH2O2<=>CH2COCH2O2H
20967.8 1.750E+003 2.560
CH2COCH2O2H<=>O(CH2)2CO+OH
25884.3 3.750E+009 1.010
CH2COCH2O2H<=>CH2CO+CH2O2H
31424.9 2.470E+011 0.480

!REF: ANALOGY WITH OXETANE<=>C2H4+CH2O.

!REF: L. ZALOTAI; Z. HUNYADI-ZOLTÁN; T. BÉRCES; F. MÁRTA, INT. J. CHEM.
KINET. 15 (6) (1983) 505-519.

O(CH2)2CO<=>CH2O+CH2CO
62022.0 2.630E+015 0.000

!REF:ANALOGY TO ETHANE

!CH3COCH3+HO2<=>CH3COCH2+H2O2
20460.0 1.700E+013 0.000
!CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H
20460.0 1.700E+013 0.000

!REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006

!CH2CO+CH3<=>CH3COCH2
6130.0 1.760E+004 2.480
!CH3COCH2+HO2<=>CH3COCH2O+OH
0.0 2.410E+013 0.000
!CH3COCH2+CH3O2<=>CH3COCH2O+CH3O
0.0 1.205E+013 0.000
!CH3COCH2+H<=>CH3COCH3
0.0 1.000E+013 0.000
!CH3COCH2O<=>CH3CO+CH2O
5108.0 5.000E+010 0.000

!REF:

!CH3COCH2+O2<=>CH3COCH2O2
-1100.0 1.200E+011 0.000

!REF:WESTBROOK ESTIMATE

!CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21 5000.0	1.000E+011	0.000
!CH2O+CH3COCH2O2<=>HCO+C3KET21 9000.0	1.288E+011	0.000
!HO2+CH3COCH2O2<=>C3KET21+O2 0.0	1.000E+012	0.000
!REF:ESTIMATE		
C2H3+HCO<=>C2H3CHO 0.0	1.810E+013	0.000
!REF:BASED ON CH3CHO+H		
C2H3CHO+H<=>C2H3CO+H2 3300.0	1.340E+013	0.000
C2H3CHO+O<=>C2H3CO+OH 1868.0	5.940E+012	0.000
!REF:TAYLOR ET AL. 1996		
C2H3CHO+OH<=>C2H3CO+H2O -962.0	9.240E+006	1.500
C2H3CHO+O2<=>C2H3CO+HO2 40700.0	1.005E+013	0.000
!REF:BASED ON CH3CHO+HO2		
C2H3CHO+HO2<=>C2H3CO+H2O2 11920.0	3.010E+012	0.000
C2H3CHO+CH3<=>C2H3CO+CH4 5911.0	2.608E+006	1.780
!REF:ANALOGY WITH ACETALDEHYDE.		
C2H3CHO+C2H3<=>C2H3CO+C2H4 8440.0	1.740E+012	0.000
!REF:ANALOGY WITH CH3CHO+CH3O		
C2H3CHO+CH3O<=>C2H3CO+CH3OH 3300.0	1.000E+012	0.000
!REF:BASED ON CH3CHO+HO2		
C2H3CHO+CH3O2<=>C2H3CO+CH3O2H 11920.0	3.010E+012	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
C2H3+CO<=>C2H3CO 4810.0	1.510E+011	0.000
!REF:		
C2H5+HCO<=>C2H5CHO 0.0	1.810E+013	0.000
!REF:ANALOGY WITH CH3CHO+H		
C2H5CHO+H<=>C2H5CO+H2 4200.0	4.000E+013	0.000
!REF:ANALOGY WITH CH3CHO+O		
C2H5CHO+O<=>C2H5CO+OH 1790.0	5.000E+012	0.000
!REF:ESTIMATE		

C2H5CHO+OH<=>C2H5CO+H2O -340.0	2.690E+010	0.760
!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98		
C2H5CHO+CH3<=>C2H5CO+CH4 5911.0	2.608E+006	1.780
!REF:ANALOGY WITH CH3CHO+HO2		
C2H5CHO+HO2<=>C2H5CO+H2O2 13600.0	2.800E+012	0.000
!REF:!ANALOGY WITH CH3CHO+CH3O		
C2H5CHO+CH3O<=>C2H5CO+CH3OH 3300.0	1.000E+012	0.000
!REF:ANALOGY WITH CH3CHO+HO2		
C2H5CHO+CH3O2<=>C2H5CO+CH3O2H 11920.0	3.010E+012	0.000
!REF:ACETALDEHYDE ANALOG		
C2H5CHO+C2H5<=>C2H5CO+C2H6 8000.0	1.000E+012	0.000
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH 3300.0	6.026E+011	0.000
!REF:BASED ON CH3CHO+HO2		
C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H 11920.0	3.010E+012	0.000
!REF:ESTIMATE		
C2H5CHO+O2<=>C2H5CO+HO2 40700.0	1.005E+013	0.000
!REF:BASED ON CH3CHO+HO2		
C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H 11920.0	3.010E+012	0.000
!REF:!ANALOGY WITH ACETALDEHYDE		
C2H5CHO+C2H3<=>C2H5CO+C2H4 8440.0	1.700E+012	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
C2H5+CO<=>C2H5CO 4810.0	1.510E+011	0.000
!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.		
CH3O+HCO<=>CH3OCHO 0.0	3.000E+013	0.000
!REF:ESTIMATE		
CH3+OCHO<=>CH3OCHO 0.0	1.000E+013	0.000
CH3OCHO+O2<=>CH3OCO+HO2 49700.0	1.000E+013	0.000
CH3OCHO+O2<=>CH2OCHO+HO2 52000.0	2.050E+013	0.000
!REF:ANOLOGY TO PROPANE		

CH3OCHO+OH<=>CH3OCO+H2O 934.0	1.580E+007	1.800
CH3OCHO+OH<=>CH2OCHO+H2O 1586.0	5.270E+009	0.970
!REF:CURRAN ESTIMATE TSANG '88 PRIMARY H		
CH3OCHO+HO2<=>CH3OCO+H2O2 13910.0	4.820E+003	2.600
!REF:CURRAN ESTIMATE TSANG '88 SECONDARY H		
CH3OCHO+HO2<=>CH2OCHO+H2O2 16490.0	2.380E+004	2.550
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+O<=>CH3OCO+OH 2830.0	2.755E+005	2.450
!REF: FIT TO COHEN/ WESTBERG '86		
CH3OCHO+O<=>CH2OCHO+OH 4750.0	9.800E+005	2.430
!REF:1/ 2 TSANG'S C3H8+H		
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+H<=>CH3OCO+H2 4471.0	6.500E+005	2.400
CH3OCHO+H<=>CH2OCHO+H2 6756.0	6.650E+005	2.540
!REF:C3H8+CH3<=>IC3H7+CH4		
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+CH3<=>CH3OCO+CH4 5481.0	7.550E-001	3.460
!REF:C3H8+CH3<=>NC3H7+CH4		
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+CH3<=>CH2OCHO+CH4 7154.0	4.520E-001	3.650
!REF:ESTIMATE		
CH3OCHO+CH3O<=>CH3OCO+CH3OH 5000.0	5.480E+011	0.000
CH3OCHO+CH3O<=>CH2OCHO+CH3OH 6458.0	2.170E+011	0.000
!REF:ANOLOGY WITH HO2		
CH3OCHO+CH3O2<=>CH3OCO+CH3O2H 13910.0	4.820E+003	2.600
CH3OCHO+CH3O2<=>CH2OCHO+CH3O2H 16490.0	2.380E+004	2.550
!REF:C3H8+HCO		
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+HCO<=>CH3OCO+CH2O 17010.0	5.400E+006	1.900

CH3OCHO+HCO<=>CH2OCHO+CH2O 1.025E+005 2.500
18430.0

!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.
CH3OCO<=>CH2OCHO 1.629E+012 -0.180
40670.0

!REF: PRIVATE COMMUNICATION FROM S.J. KLIPPENSTEIN
CH3OCO<=>CH3+CO2 8.691E+017 -1.810
13656.7

PLOG/ 0.0500 9.720E+012 -1.310 9416.7/
PLOG/ 1.0000 1.250E+016 -1.830 11340.8/
PLOG/ 10.0000 1.040E+018 -2.100 12826.9/
PLOG/ 100.0000 8.690E+017 -1.810 13656.7/
CH3OCO<=>CH3O+CO 8.691E+017 -1.810
13656.7
PLOG/ 0.0500 1.030E+003 1.290 25401.0/
PLOG/ 1.0000 4.090E+005 0.810 21969.1/
PLOG/ 10.0000 9.020E+014 -1.720 21767.5/
PLOG/ 100.0000 2.825E+022 -3.440 23592.4/

!REF:PIERRE GLAUDE'S RATES

!REF: CURRAN ESTIMATE
CH2O+HCO<=>CH2OCHO 1.500E+011 0.000
11900.0

!REF:OEHSCHLAEGER ET AL., PROC COMB INST 30 (2005) 1119-1127
C3H8 (+M) <=>CH3+C2H5 (+M) 1.290E+037 -5.840
97380.0
LOW/ 5.640E+074 -15.740
98714.0/
TROE/ 3.100E-001 5.000E+001 3.000E+003 9.000E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/

!REF:ESTIMATE
NC3H7+H<=>C3H8 1.000E+014 0.000
0.0

!REF:ESTIMATE
IC3H7+H<=>C3H8 1.000E+014 0.000
0.0

!REF:
C3H8+O2<=>IC3H7+HO2 2.000E+013 0.000
49640.0
C3H8+O2<=>NC3H7+HO2 6.000E+013 0.000
52290.0
H+C3H8<=>H2+IC3H7 1.300E+006 2.400
4471.0
H+C3H8<=>H2+NC3H7 3.490E+005 2.690
6450.0
C3H8+O<=>IC3H7+OH 5.490E+005 2.500
3140.0
C3H8+O<=>NC3H7+OH 3.710E+006 2.400
5505.0

C3H8+OH<=>NC3H7+H2O 1586.0	1.054E+010	0.970
C3H8+OH<=>IC3H7+H2O -35.0	4.670E+007	1.610
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C3H8+HO2<=>IC3H7+H2O2 13720.0	6.320E+001	3.370
C3H8+HO2<=>NC3H7+H2O2 17160.0	4.080E+001	3.590
!REF:FIT TO NIST DATABASE		
CH3+C3H8<=>CH4+IC3H7 7520.0	6.400E+004	2.170
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3+C3H8<=>CH4+NC3H7 7154.0	9.040E-001	3.650
!REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L.,		
!REF:AND GLASSMAN, I., TO BE PUBLISHED.		
IC3H7+C3H8<=>NC3H7+C3H8 12900.0	3.000E+010	0.000
C2H3+C3H8<=>C2H4+IC3H7 10400.0	1.000E+011	0.000
C2H3+C3H8<=>C2H4+NC3H7 10400.0	1.000E+011	0.000
C2H5+C3H8<=>C2H6+IC3H7 10400.0	1.000E+011	0.000
C2H5+C3H8<=>C2H6+NC3H7 10400.0	1.000E+011	0.000
!REF:DAGAUT ET AL., CST 71, 111(1990)		
C3H8+C3H5-A<=>NC3H7+C3H6 20500.0	7.940E+011	0.000
C3H8+C3H5-A<=>IC3H7+C3H6 16200.0	7.940E+011	0.000
!REF:DRYER ESTIMATE		
C3H8+CH3O<=>NC3H7+CH3OH 7000.0	3.000E+011	0.000
C3H8+CH3O<=>IC3H7+CH3OH 7000.0	3.000E+011	0.000
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
!REF:SCALED AS PER CARSTENSEN ET AL		
CH3O2+C3H8<=>CH3O2H+NC3H7 18280.0	1.386E+000	3.970
CH3O2+C3H8<=>CH3O2H+IC3H7 14810.0	1.019E+001	3.580
C2H5O2+C3H8<=>C2H5O2H+NC3H7 18280.0	1.386E+000	3.970
C2H5O2+C3H8<=>C2H5O2H+IC3H7 14810.0	1.019E+001	3.580

!REF:ANALOGY TO C2H6+HO2
NC3H7O2+C3H8<=>NC3H7O2H+NC3H7
20460.0 1.700E+013 0.000

!REF:WALKER, R. W., REACTION KINETICS,

!REF:VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975
NC3H7O2+C3H8<=>NC3H7O2H+IC3H7
17000.0 2.000E+012 0.000

!REF:ANALOGY TO C2H6+HO2
IC3H7O2+C3H8<=>IC3H7O2H+NC3H7
20460.0 1.700E+013 0.000

!REF:WALKER, R. W., REACTION KINETICS,

!REF:VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975
IC3H7O2+C3H8<=>IC3H7O2H+IC3H7
17000.0 2.000E+012 0.000

C3H8+CH3CO3<=>IC3H7+CH3CO3H
17000.0 2.000E+012 0.000

!REF:ANALOGY TO C2H6+HO2
C3H8+CH3CO3<=>NC3H7+CH3CO3H
20460.0 1.700E+013 0.000

C3H8+O2CHO<=>NC3H7+HO2CHO
16480.0 5.520E+004 2.550

C3H8+O2CHO<=>IC3H7+HO2CHO
13910.0 1.475E+004 2.600

!REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006

!REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST
IC3H7+H<=>C2H5+CH3
0.0 2.000E+013 0.000

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
IC3H7+OH<=>C3H6+H2O
0.0 2.410E+013 0.000

IC3H7+O<=>CH3COCH3+H
0.0 4.818E+013 0.000

IC3H7+O<=>CH3CHO+CH3
0.0 4.818E+013 0.000

!REF:REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006
NC3H7+O2<=>C3H6+HO2
3000.0 3.000E-019 0.000

!REF:ANALOGY WITH ACETALDEHYDE
C2H5CHO+NC3H7<=>C2H5CO+C3H8
8440.0 1.700E+012 0.000

C2H5CHO+IC3H7<=>C2H5CO+C3H8
8440.0 1.700E+012 0.000

C2H5CHO+C3H5-A<=>C2H5CO+C3H6
8440.0 1.700E+012 0.000

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C2H3+CH3 (+M) <=>C3H6 (+M)	2.500E+013	0.000
0.0		
LOW/	4.270E+058	-11.940
9769.8/		
TROE/ 1.750E-001 1.341E+003 6.000E+004 1.014E+004/		
C3H5-A+H (+M) <=>C3H6 (+M)	1.000E+014	0.000
0.0		
LOW/	6.650E+059	-12.000
5967.8/		
TROE/ 2.000E-002 1.097E+003 1.097E+003 6.860E+003/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/		
0.70/		
C3H6<=>C3H5-S+H	7.710E+069	-16.090
140000.0		
C3H6<=>C3H5-T+H	5.620E+071	-16.580
139300.0		

!REF:!FROM KOERT ET AL. ENERGY & FUELS VOL 6: 485-493 1992

!REF: ANALOGY WITH C2H4

C3H6+O<=>C2H5+HCO	7.450E+006	1.880
183.0		
C3H6+O=>CH2CO+CH3+H	3.050E+006	1.880
183.0		
C3H6+O=>CH3CHCO+H+H	3.050E+006	1.880
183.0		
C3H6+O<=>C3H5-A+OH	5.240E+011	0.700
5884.0		
C3H6+O<=>C3H5-S+OH	1.200E+011	0.700
8959.1		
C3H6+O<=>C3H5-T+OH	6.030E+010	0.700
7632.0		
C3H6+OH<=>C3H5-A+H2O	4.460E+006	2.072
1050.8		
C3H6+OH<=>C3H5-S+H2O	1.860E+005	2.369
2502.0		
C3H6+OH<=>C3H5-T+H2O	1.800E+006	1.979
2235.2		

!REF:BILL

!REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONDARY ALKYL AND PRIMARY ALLYLIC WITH F<=>.2: 0.2 (98.4-88.2) <=>.2*10.2<=>2.0

C3H6+CH3O<=>C3H5-A+CH3OH	8.400E+010	0.000
2600.0		

!REF: C3 NUIG CALCULATION J.M

C3H6+HO2<=>C3H5-S+H2O2	9.570E+002	3.059
20798.6		
C3H6+HO2<=>C3H5-T+H2O2	1.560E+004	2.820
24427.9		
C3H6+HO2<=>IC3H7O2	1.050E-025	3.520
5109.0		
PLOG/ 0.0130 8.280E+054 -14.710 21141.0/		
PLOG/ 0.9869 1.170E+042 -10.250 18891.0/		
PLOG/ 9.8700 1.170E+038 -8.770 18811.0/		
PLOG/ 98.6900 5.570E+022 -3.910 13896.0/		

C3H6+HO2<=>C3H6OOH2-1				4.850E-021	2.650
11201.0					
PLOG/	0.0130	1.310E+013	-1.840	8561.0/	
PLOG/	0.9869	5.930E+017	-2.610	11533.0/	
PLOG/	9.8700	8.340E+024	-4.400	16440.0/	
PLOG/	98.6900	3.750E+023	-3.680	17965.0/	
C3H6+HO2<=>C3H6O1-2+OH				1.130E+019	-1.680
23587.0					
PLOG/	0.0130	3.730E+003	2.640	11173.0/	
PLOG/	0.9869	1.780E+012	0.110	16137.0/	
PLOG/	9.8700	3.900E+017	-1.400	20077.0/	
PLOG/	98.6900	1.130E+019	-1.680	23587.0/	
C3H6+HO2<=>IC3H7+O2				8.870E+022	-3.090
26586.0					
PLOG/	0.0130	1.020E+007	1.160	10273.0/	
PLOG/	0.9869	1.310E+020	-2.580	19078.0/	
PLOG/	9.8700	4.140E+028	-4.920	26212.0/	
PLOG/	98.6900	8.870E+022	-3.090	26586.0/	
C3H6OOH2-1<=>C3H6O1-2+OH				6.910E+007	1.370
13373.0					
PLOG/	0.0130	2.660E+035	-8.360	18056.0/	
PLOG/	0.9869	1.960E+035	-7.660	20595.0/	
PLOG/	9.8700	2.240E+033	-6.750	21619.0/	
PLOG/	98.6900	8.480E+026	-4.580	20278.0/	
C3H6+HO2<=>C3H5-A+H2O2				3.070E-002	4.403
13547.2					

!REF:LASKIN ET AL IJCK 32 589-614 2000

!REF: CURRAN EST

C3H6+H<=>NC3H7				1.000E+000	1.000
0.0					
PLOG/	0.0013	7.990E+081	-23.161	22239.0/	
PLOG/	0.0400	4.240E+068	-18.427	19665.0/	
PLOG/	1.0000	1.040E+049	-11.500	15359.0/	
PLOG/	10.0000	6.200E+041	-8.892	14637.0/	
!PLOG/	100.0000	-6.450E+031	-5.851	8177.8/	
DUP					
C3H6+H<=>NC3H7				1.000E+000	1.000
0.0					
PLOG/	0.0013	1.850E+026	-5.830	3865.8/	
PLOG/	0.0400	2.820E+030	-6.490	5470.8/	
PLOG/	1.0000	3.780E+028	-5.570	5625.1/	
PLOG/	10.0000	1.460E+025	-4.280	5247.8/	
!REF: REFIT TO ONE PARAMETER TO AVOID PROBLEMS WITH NEGATIVE K					
PLOG/	100.0000	4.220E+027	-4.390	9345.8/	
DUP					
C3H6+H<=>C2H4+CH3				1.000E+000	1.000
1.0					
PLOG/	0.0013	1.540E+009	1.350	2542.0/	
PLOG/	0.0400	7.880E+010	0.870	3599.6/	
PLOG/	1.0000	2.670E+012	0.470	5431.1/	
PLOG/	10.0000	9.250E+022	-2.600	12898.0/	
PLOG/	100.0000	1.320E+023	-2.420	16500.0/	
DUP					
C3H6+H<=>C2H4+CH3				1.000E+000	1.000
1.0					
PLOG/	10.0000	1.240E+005	2.520	3679.1/	

PLOG/	100.0000	2.510E+003	2.910	3980.9/	
DUP					
C3H6+H<=>IC3H7				1.000E+000	1.000
1.0					
PLOG/	0.0013	1.350E+044	-10.680	8196.4/	
PLOG/	0.0400	2.110E+057	-14.230	15147.0/	
PLOG/	1.0000	3.260E+061	-14.940	20161.0/	
PLOG/	10.0000	5.300E+056	-13.120	20667.0/	
PLOG/	100.0000	1.110E+050	-10.800	20202.0/	
DUP					
C3H6+H<=>IC3H7				1.000E+000	1.000
1.0					
PLOG/	0.0013	2.170E+130	-32.580	136140.0/	
PLOG/	0.0400	2.250E+029	-5.840	4241.9/	
PLOG/	1.0000	1.060E+030	-5.630	5613.4/	
PLOG/	10.0000	6.110E+026	-4.440	5182.3/	
PLOG/	100.0000	2.730E+023	-3.260	4597.0/	
DUP					
C2H4+CH3<=>NC3H7				1.000E+000	1.000
1.0					
PLOG/	0.0013	8.670E+048	-12.540	18206.0/	
PLOG/	0.0400	1.060E+049	-12.040	20001.0/	
PLOG/	1.0000	7.670E+047	-11.170	22366.0/	
PLOG/	10.0000	1.810E+045	-10.030	23769.0/	
PLOG/	100.0000	2.040E+040	-8.250	24214.0/	
DUP					
C2H4+CH3<=>NC3H7				1.000E+000	1.000
1.0					
PLOG/	0.0013	1.120E+043	-11.300	13080.0/	
PLOG/	0.0400	7.280E+039	-9.880	13164.0/	
PLOG/	1.0000	2.600E+033	-7.460	12416.0/	
PLOG/	10.0000	3.850E+027	-5.380	11455.0/	
PLOG/	100.0000	1.660E+021	-3.170	10241.0/	
DUP					
C3H6+H<=>C3H5-A+H2				3.644E+005	2.455
4361.2					
C3H6+H<=>C3H5-T+H2				1.498E+002	3.381
8909.5					
C3H6+H<=>C3H5-S+H2				5.101E+002	3.234
12357.0					
DUP					
C3H6+H<=>C3H5-S+H2				3.969E+002	3.252
12007.0					
DUP					
C2H4+CH3<=>C2H3+CH4				9.760E+002	2.947
15148.0					
DUP					
C2H4+CH3<=>C2H3+CH4				8.130E-005	4.417
8835.8					
DUP					

!REF:LASKIN ET AL IJCK 32 589-614 2000

!REF:ORIGINAL:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.

!REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346

C3H5-A+HO2<=>C3H5O+OH				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.020E+013	-0.158	-1417.0/	
PLOG/	0.1000	4.980E+014	-0.642	-349.1/	
PLOG/	1.0000	7.770E+017	-1.520	2379.2/	
PLOG/	10.0000	2.930E+015	-0.684	3615.3/	
PLOG/	100.0000	1.640E+004	2.740	1144.4/	
C3H5-A+HO2<=>AC3H5OOH				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.910E+031	-7.230	1336.2/	
PLOG/	0.1000	6.310E+042	-10.300	5568.9/	
PLOG/	1.0000	1.030E+045	-10.600	7851.5/	
PLOG/	10.0000	2.790E+037	-7.920	6497.9/	
PLOG/	100.0000	4.730E+025	-4.130	2923.8/	
C3H5-A+HO2<=>C2H3CHO+H2O				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.090E+000	3.010	-3421.1/	
PLOG/	0.1000	6.350E+001	2.500	-2341.4/	
PLOG/	1.0000	6.050E+005	1.390	595.1/	
PLOG/	10.0000	3.100E+005	1.590	2677.6/	
PLOG/	100.0000	5.070E-005	4.590	927.5/	
AC3H5OOH<=>C2H3CHO+H2O				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.990E+050	-12.700	53531.9/	
PLOG/	0.1000	4.720E+047	-11.500	54360.9/	
PLOG/	1.0000	1.500E+040	-8.840	53179.2/	
PLOG/	10.0000	2.540E+028	-5.000	49919.4/	
PLOG/	100.0000	1.480E+016	-1.120	45949.3/	
AC3H5OOH<=>C3H5O+OH				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.490E+058	-13.900	54266.9/	
PLOG/	0.1000	1.800E+054	-12.400	54193.8/	
PLOG/	1.0000	3.360E+046	-9.810	52468.5/	
PLOG/	10.0000	2.390E+036	-6.540	49429.0/	
PLOG/	100.0000	1.280E+027	-3.610	46333.1/	
C3H5O<=>C2H3+CH2O				1.000E+011	0.000
0.0					
PLOG/	0.0010	7.260E+006	0.182	17815.5/	
PLOG/	0.0100	6.970E+016	-2.500	20878.7/	
PLOG/	0.1000	6.640E+023	-4.230	23565.0/	
PLOG/	1.0000	1.070E+026	-4.560	24622.9/	
PLOG/	10.0000	6.500E+029	-5.370	26645.0/	
PLOG/	100.0000	4.630E+031	-5.590	28915.3/	
PLOG/	1000.0000	8.520E+025	-3.610	27863.4/	
C3H5O<=>C2H3OCH2				1.000E+011	0.000
0.0					
PLOG/	0.0010	3.170E+020	-4.150	12121.3/	
PLOG/	0.0100	4.790E+024	-5.030	14606.1/	
PLOG/	0.1000	1.900E+026	-5.160	16124.4/	
PLOG/	1.0000	1.510E+028	-5.400	18165.4/	
PLOG/	10.0000	2.420E+028	-5.170	19691.2/	
PLOG/	100.0000	5.570E+024	-3.860	19395.2/	
PLOG/	1000.0000	1.350E+018	-1.730	17386.5/	
C3H5O<=>CH2CH2CHO				1.000E+011	0.000
0.0					
PLOG/	0.0010	5.250E-049	15.500	-15639.9/	
PLOG/	0.0100	1.460E-088	27.600	-35995.0/	
PLOG/	0.1000	4.440E-022	8.380	-3819.0/	

PLOG/	1.0000	6.230E+012	-1.440	10829.2/	
PLOG/	10.0000	3.480E+042	-9.910	25297.9/	
PLOG/	100.0000	1.880E+038	-8.160	25974.5/	
PLOG/	1000.0000	1.670E+021	-2.740	20337.7/	
C3H5O<=>C2H3CHO+H				1.000E+011	0.000
0.0					
PLOG/	0.0010	3.000E+015	-2.310	14667.9/	
PLOG/	0.0100	1.500E+022	-3.960	18283.0/	
PLOG/	0.1000	1.950E+023	-3.990	19143.3/	
PLOG/	1.0000	1.150E+025	-4.240	20311.2/	
PLOG/	10.0000	1.760E+028	-4.890	22765.2/	
PLOG/	100.0000	1.410E+027	-4.280	23770.6/	
PLOG/	1000.0000	2.570E+020	-2.060	22040.1/	
C3H5O<=>C2H4+HCO				1.000E+011	0.000
0.0					
PLOG/	0.0010	6.620E+016	-2.840	13197.0/	
PLOG/	0.0100	1.260E+020	-3.530	15469.2/	
PLOG/	0.1000	2.130E+021	-3.640	16584.5/	
PLOG/	1.0000	1.070E+024	-4.160	18985.0/	
PLOG/	10.0000	8.420E+025	-4.400	22382.6/	
PLOG/	100.0000	1.860E+021	-2.730	23658.8/	
PLOG/	1000.0000	4.750E+008	1.140	20922.5/	
C2H3OCH2<=>C2H3+CH2O				1.000E+011	0.000
0.0					
PLOG/	0.0010	3.300E+009	-0.638	19747.8/	
PLOG/	0.0100	3.360E+021	-3.900	23945.2/	
PLOG/	0.1000	2.910E+029	-5.900	27249.7/	
PLOG/	1.0000	1.830E+034	-6.940	30690.4/	
PLOG/	10.0000	9.720E+033	-6.500	33002.5/	
PLOG/	100.0000	2.680E+027	-4.260	33305.6/	
PLOG/	1000.0000	8.810E+014	-0.326	31553.1/	
C2H3OCH2<=>CH2CH2CHO				1.000E+011	0.000
0.0					
PLOG/	0.0010	8.010E-092	27.800	-37321.2/	
PLOG/	0.0100	7.780E-011	3.700	-2766.9/	
PLOG/	0.1000	5.110E+015	-2.760	15937.6/	
PLOG/	1.0000	4.480E+025	-5.200	21532.2/	
PLOG/	10.0000	3.970E+034	-7.410	28116.9/	
PLOG/	100.0000	5.620E+022	-3.560	25806.7/	
PLOG/	1000.0000	2.510E+020	-2.630	29288.4/	
C2H3OCH2<=>C2H3CHO+H				1.000E+011	0.000
0.0					
PLOG/	0.0010	4.930E+024	-5.050	20108.4/	
PLOG/	0.0100	2.140E+028	-5.800	22219.4/	
PLOG/	0.1000	1.930E+032	-6.640	25108.2/	
PLOG/	1.0000	8.600E+034	-7.110	28209.1/	
PLOG/	10.0000	2.170E+034	-6.640	30647.6/	
PLOG/	100.0000	4.170E+028	-4.710	31231.9/	
PLOG/	1000.0000	3.980E+018	-1.620	30129.8/	
C2H3OCH2<=>C2H4+HCO				1.000E+011	0.000
0.0					
PLOG/	0.0010	8.230E+026	-5.840	19356.9/	
PLOG/	0.0100	1.320E+029	-6.210	21293.6/	
PLOG/	0.1000	3.470E+032	-6.960	24197.3/	
PLOG/	1.0000	1.440E+036	-7.760	28007.8/	
PLOG/	10.0000	9.720E+037	-8.020	32394.6/	
PLOG/	100.0000	2.430E+031	-5.810	34295.8/	
PLOG/	1000.0000	3.730E+014	-0.726	32008.3/	

CH2CH2CHO<=>C2H3+CH2O				1.000E+011	0.000
0.0					
PLOG/	0.0010	6.890E-069	21.500	2638.0/	
PLOG/	0.0100	5.340E-033	11.100	16749.1/	
PLOG/	0.1000	6.110E+026	-6.010	44116.7/	
PLOG/	1.0000	8.040E+035	-8.310	46919.7/	
PLOG/	10.0000	5.520E+040	-9.190	50508.7/	
PLOG/	100.0000	5.850E+035	-7.180	52038.4/	
PLOG/	1000.0000	1.930E+019	-1.940	48440.0/	
CH2CH2CHO<=>C2H3CHO+H				1.000E+011	0.000
0.0					
PLOG/	0.0010	1.610E+010	-1.240	32371.3/	
PLOG/	0.0100	5.840E+015	-2.610	32878.4/	
PLOG/	0.1000	3.640E+023	-4.600	34275.3/	
PLOG/	1.0000	7.580E+031	-6.630	37895.4/	
PLOG/	10.0000	2.860E+032	-6.300	39990.7/	
PLOG/	100.0000	1.570E+023	-3.140	38011.7/	
PLOG/	1000.0000	4.520E+012	0.214	34570.5/	
CH2CH2CHO<=>C2H4+HCO				1.000E+011	0.000
0.0					
PLOG/	0.0010	2.900E+032	-7.240	25687.5/	
PLOG/	0.0100	5.300E+033	-7.280	27100.6/	
PLOG/	0.1000	2.000E+035	-7.410	29027.3/	
PLOG/	1.0000	1.010E+034	-6.700	30018.1/	
PLOG/	10.0000	9.760E+027	-4.630	28923.9/	
PLOG/	100.0000	2.110E+019	-1.850	26239.8/	
PLOG/	1000.0000	1.590E+013	0.063	24086.3/	
C2H3+CH2O<=>C2H3CHO+H				1.000E+011	0.000
0.0					
PLOG/	0.0010	2.600E+004	2.260	1510.3/	
PLOG/	0.0100	5.130E+004	2.170	1675.5/	
PLOG/	0.1000	3.990E+005	1.910	2218.3/	
PLOG/	1.0000	1.750E+007	1.450	3428.0/	
PLOG/	10.0000	1.350E+009	0.933	5173.0/	
PLOG/	100.0000	2.240E+011	0.357	8001.3/	
PLOG/	1000.0000	6.010E+005	2.090	7895.6/	
C2H3+CH2O<=>C2H4+HCO				1.000E+011	0.000
0.0					
PLOG/	0.0010	1.110E+007	1.090	1807.2/	
PLOG/	0.0100	2.470E+007	0.993	1994.9/	
PLOG/	0.1000	2.470E+008	0.704	2596.2/	
PLOG/	1.0000	1.420E+010	0.209	3934.2/	
PLOG/	10.0000	3.450E+013	-0.726	6944.3/	
PLOG/	100.0000	3.310E+014	-0.866	10965.7/	
PLOG/	1000.0000	1.650E+001	3.170	9399.8/	
!REF: ESTIMATE C3 NUIG S. M. BURKE					
C3H6+O2<=>C3H5-A+HO2				5.960E+019	-1.670
46192.1					
C3H6+O2<=>C3H5-S+HO2				2.000E+013	0.000
62270.0					
C3H6+O2<=>C3H5-T+HO2				1.000E+013	0.000
58770.0					
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)					
C3H6+CH3<=>C3H5-A+CH4				2.210E+000	3.500
5675.0					

C3H6+CH3<=>C3H5-S+CH4	1.348E+000	3.500		
12850.0				
C3H6+CH3<=>C3H5-T+CH4	8.400E-001	3.500		
11660.0				
!REF:!ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)				
C3H6+C2H5<=>C3H5-A+C2H6	1.000E+011	0.000		
9800.0				
!REF:ANALOGY TO C3H6+HO2				
C3H6+CH3O2<=>C3H5-A+CH3O2H	7.680E-002	4.403		
13547.2				
C3H6+CH3CO3<=>C3H5-A+CH3CO3H	7.680E-002	4.403		
13547.2				
!REF:				
!REF:ANALOGY TO C3H6+HO2				
C3H6+C2H5O2<=>C3H5-A+C2H5O2H	7.680E-002	4.403		
13547.2				
C3H6+NC3H7O2<=>C3H5-A+NC3H7O2H	7.680E-002	4.403		
13547.2				
C3H6+IC3H7O2<=>C3H5-A+IC3H7O2H	7.680E-002	4.403		
13547.2				
!REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053				
C3H6+OH<=>C3H5OH+H	2.290E+013	0.070		
10580.0				
PLOG/	0.0013	2.670E+013	0.050	10611.0/
PLOG/	0.0100	2.750E+013	0.050	10623.0/
PLOG/	0.0130	2.870E+013	0.040	10634.0/
PLOG/	0.0250	1.590E+014	-0.160	11125.0/
PLOG/	0.1000	3.100E+014	-0.220	11407.0/
PLOG/	0.1315	3.780E+014	-0.240	11458.0/
PLOG/	1.0000	9.150E+007	1.420	10087.0/
PLOG/	10.0000	3.660E+005	2.140	10410.0/
PLOG/	100.0000	8.190E+002	2.840	10481.0/
C3H6+OH<=>C2H3OH+CH3	1.290E+006	1.650		
1233.0				
PLOG/	0.0013	1.290E+006	1.650	1233.0/
PLOG/	0.0100	1.820E+004	2.100	1162.0/
PLOG/	0.0130	2.040E+003	2.480	1128.0/
PLOG/	0.0250	2.880E+002	2.800	1152.0/
PLOG/	0.1000	1.400E+001	3.210	1208.0/
PLOG/	0.1315	7.710E+000	3.290	1216.0/
PLOG/	1.0000	1.130E+004	2.500	3238.0/
PLOG/	10.0000	2.410E+019	-1.740	13107.0/
PLOG/	100.0000	3.300E-001	3.700	3665.0/
C3H6+OH<=>IC3H5OH+H	2.870E+000	2.920		
625.0				
PLOG/	0.0013	2.870E+000	2.920	625.0/
PLOG/	0.0100	4.840E-001	2.980	704.0/
PLOG/	0.0130	3.130E-001	3.040	721.0/
PLOG/	0.0250	9.330E-003	3.620	677.0/
PLOG/	0.1000	4.640E-005	4.480	687.0/
PLOG/	0.1315	2.710E-005	4.560	707.0/
PLOG/	1.0000	7.650E-007	5.050	874.0/
PLOG/	10.0000	2.640E+015	-0.800	12728.0/

PLOG/	100.0000	4.870E-004	4.320	4020.0/	
C3H6+OH<=>SC3H5OH+H				2.870E+000	2.920
625.0					
PLOG/	0.0013	2.870E+000	2.920	625.0/	
PLOG/	0.0100	4.840E-001	2.980	704.0/	
PLOG/	0.0130	3.130E-001	3.040	721.0/	
PLOG/	0.0250	9.330E-003	3.620	677.0/	
PLOG/	0.1000	4.640E-005	4.480	687.0/	
PLOG/	0.1315	2.710E-005	4.560	707.0/	
PLOG/	1.0000	7.650E-007	5.050	874.0/	
PLOG/	10.0000	2.640E+015	-0.800	12728.0/	
PLOG/	100.0000	4.870E-004	4.320	4020.0/	
C3H6+OH<=>CH3CHO+CH3				6.930E+005	1.490
-536.0					
PLOG/	0.0013	6.930E+005	1.490	-536.0/	
PLOG/	0.0100	5.940E+003	2.010	-560.0/	
PLOG/	0.0130	1.100E+003	2.220	-680.0/	
PLOG/	0.0250	1.070E+002	2.500	-759.0/	
PLOG/	0.1000	7.830E-001	3.100	-919.0/	
PLOG/	0.1315	3.070E-001	3.220	-946.0/	
PLOG/	1.0000	3.160E-004	4.050	-1144.0/	
PLOG/	10.0000	7.590E-006	4.490	-680.0/	
PLOG/	100.0000	5.450E-005	4.220	1141.0/	
C3H6+OH<=>C3H6OH1-2				5.100E+054	-20.700
32402.0					
PLOG/	0.0013	2.300E+078	-20.700	32402.0/	
PLOG/	0.0100	2.740E+077	-20.000	33874.0/	
PLOG/	0.0130	1.070E+076	-19.580	32874.0/	
PLOG/	0.0250	3.680E+073	-18.790	31361.0/	
PLOG/	0.1000	1.040E+068	-17.010	27909.0/	
PLOG/	0.1315	7.230E+066	-16.640	27162.0/	
PLOG/	1.0000	1.950E+059	-14.170	23079.0/	
PLOG/	10.0000	7.580E+053	-12.230	22976.0/	
PLOG/	100.0000	1.430E+048	-10.230	23772.0/	
DUP					
C3H6+OH<=>C3H6OH1-2				1.420E+036	-15.840
11594.0					
PLOG/	0.0013	6.410E+059	-15.840	11594.0/	
PLOG/	0.0100	7.280E+059	-15.510	12898.0/	
PLOG/	0.0130	2.790E+059	-15.340	12913.0/	
PLOG/	0.0250	2.650E+058	-14.930	12936.0/	
PLOG/	0.1000	1.350E+056	-14.040	12945.0/	
PLOG/	0.1315	3.980E+055	-13.850	12887.0/	
PLOG/	1.0000	1.550E+050	-12.040	11493.0/	
PLOG/	10.0000	6.410E+041	-9.350	8921.0/	
PLOG/	100.0000	2.300E+032	-6.310	6088.0/	
DUP					
C3H6+OH<=>C3H6OH2-1				5.100E+054	-20.700
32402.0					
PLOG/	0.0013	2.140E+059	-15.840	11594.0/	
PLOG/	0.0100	2.430E+059	-15.510	12898.0/	
PLOG/	0.0130	9.300E+058	-15.340	12913.0/	
PLOG/	0.0250	8.830E+057	-14.930	12936.0/	
PLOG/	0.1000	4.500E+055	-14.040	12945.0/	
PLOG/	0.1315	1.330E+055	-13.850	12887.0/	
PLOG/	1.0000	5.180E+049	-12.040	11493.0/	
PLOG/	10.0000	2.140E+041	-9.350	8921.0/	
PLOG/	100.0000	7.650E+031	-6.310	6088.0/	

PLOG/	200	1.32E+12	-0.25	10285/		
DUP						
C3H6OH1-2+O2<=>SC3H5OH+HO2		1.420E+036	-15.840		11594.0	
PLOG/	0.001	3.22E+23	-4.69	5341/		
PLOG/	0.01	4.80E+28	-6.18	8461/		
PLOG/	0.1	1.71E+32	-7.16	11410/		
PLOG/	1	1.53E+32	-7.02	13378/		
PLOG/	10	5.55E+29	-6.14	15100/		
PLOG/	40	1.72E+26	-4.97	15849/		
PLOG/	100	4.46E+21	-3.51	15644/		
PLOG/	200	5.06E+16	-1.96	14979/		
DUP						
C3H6OH1-2+O2<=>TQC3H6OI		1.420E+036	-15.840		11594.0	
PLOG/	0.001	6.36+104	-33.74	22390/		
PLOG/	0.01	7.96+103	-33.01	22966/		
PLOG/	0.1	6.99E+96	-30.48	20584/		
PLOG/	1	1.04E+88	-27.47	16629/		
PLOG/	10	3.13E+96	-29.62	20346/		
PLOG/	40	2.79+105	-32.04	24971/		
PLOG/	100	4.64+109	-33.12	27657/		
PLOG/	200	2.06+111	-33.48	29197/		
C3H6OH1-2+O2<=>CH3CHO+CH2O+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	3.03E+37	-8.35	6940/		
PLOG/	0.01	1.07E+42	-9.64	9965/		
PLOG/	0.1	9.22E+43	-10.12	12427/		
PLOG/	1	1.14E+42	-9.42	13806/		
PLOG/	10	1.80E+38	-8.13	15131/		
PLOG/	40	1.61E+34	-6.8	15691/		
PLOG/	100	7.00E+29	-5.41	15552/		
PLOG/	200	3.74E+25	-4.06	15118/		
C3H6OH1-2+O2<=>QC3H5OHP		1.420E+036	-15.840		11594.0	
PLOG/	0.001	1.18+118	-37.6	26229 /		
PLOG/	0.01	1.91+131	-40.73	34079/		
PLOG/	0.1	5.81+138	-42.17	40750/		
PLOG/	1	5.05+134	-40.19	43580/		
PLOG/	10	2.07+117	-34.26	41516/		
PLOG/	40	1.71+101	-29.04	38094/		
PLOG/	100	1.25E+89	-25.15	35203/		
PLOG/	200	2.98E+79	-22.09	32802/		
C3H6OH1-2+O2<=>CY(COC)COH+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	2.11E+18	-2.87	6870/		
PLOG/	0.01	3.02E+27	-5.54	11842/		
PLOG/	0.1	1.36E+37	-8.29	18165/		
PLOG/	1	1.21E+39	-8.66	22517/		
PLOG/	10	1.53E+28	-5.13	22530/		
PLOG/	40	2.72E+15	-1.16	20283/		
PLOG/	100	1.06E+05	2.06	18044/		
PLOG/	200	2.30E-04	4.73	16037/		
C3H6OH1-2+O2<=>TQC3H5OHI		1.420E+036	-15.840		11594.0	
PLOG/	0.001	1.76E+53	-19.87	9019/		
PLOG/	0.01	4.68E+67	-23.92	11892/		
PLOG/	0.1	2.07E+91	-30.58	17347/		
PLOG/	1	2.84+100	-32.4	20041/		
PLOG/	10	1.16+115	-35.81	27656/		
PLOG/	40	4.87+123	-37.83	33314/		
PLOG/	100	7.95+124	-37.82	35683/		
PLOG/	200	4.58+122	-36.86	36374/		
C3H6OH1-2+O2<=>CCY(COC)OH+OH		1.420E+036	-15.840		11594.0	

PLOG/	0.001	1.42E+32	-6.95	6210/		
PLOG/	0.01	5.19E+36	-8.24	9233/		
PLOG/	0.1	5.77E+38	-8.76	11715/		
PLOG/	1	2.86E+36	-7.95	12823/		
PLOG/	10	1.37E+32	-6.51	13646/		
PLOG/	40	2.15E+29	-5.56	14541/		
PLOG/	100	1.20E+26	-4.51	14778/		
PLOG/	200	3.31E+22	-3.37	14606/		
TQJC3H6OH<=>C3H5OH+HO2		1.420E+036	-15.840		11594.0	
PLOG/	0.001	9.73E+65	-18.5	42975/		
PLOG/	0.01	1.04E+64	-17.25	44419/		
PLOG/	0.1	7.90E+59	-15.59	44504/		
PLOG/	1	9.35E+53	-13.49	43566/		
PLOG/	10	4.13E+44	-10.39	41279/		
PLOG/	40	6.57E+38	-8.49	39745/		
PLOG/	100	8.32E+34	-7.23	38675/		
PLOG/	200	9.46E+31	-6.28	37849/		
DUP						
TQJC3H6OH<=>C3H5OH+HO2		1.420E+036	-15.840		11594.0	
PLOG/	0.001	5.27E+64	-18	42872/		
PLOG/	0.01	4.82E+62	-16.74	44284/		
PLOG/	0.1	3.42E+58	-15.07	44348/		
PLOG/	1	4.05E+52	-12.97	43402/		
PLOG/	10	1.93E+43	-9.88	41120/		
PLOG/	40	3.28E+37	-7.99	39593/		
PLOG/	100	4.35E+33	-6.74	38527/		
PLOG/	200	5.13E+30	-5.79	37706/		
DUP						
TQJC3H6OH<=>TQC3H6OI		1.420E+036	-15.840		11594.0	
PLOG/	0.001	3.78E+50	-12.91	31539/		
PLOG/	0.01	1.42E+45	-10.94	30864/		
PLOG/	0.1	1.50E+40	-9.21	29932/		
PLOG/	1	3.12E+35	-7.64	28864/		
PLOG/	10	2.73E+29	-5.67	27243/		
PLOG/	40	8.88E+25	-4.54	26272/		
PLOG/	100	4.60E+23	-3.8	25622/		
PLOG/	200	9.08E+21	-3.25	25131/		
TQJC3H6OH<=>QC3H5OHP		1.420E+036	-15.840		11594.0	
PLOG/	0.001	9.16E+62	-18.02	45297/		
PLOG/	0.01	2.56E+62	-17.1	47393/		
PLOG/	0.1	1.25E+59	-15.61	47984/		
PLOG/	1	1.97E+53	-13.49	47281/		
PLOG/	10	1.91E+43	-10.15	44926/		
PLOG/	40	7.68E+36	-8.05	43267/		
PLOG/	100	3.49E+32	-6.64	42089/		
PLOG/	200	1.77E+29	-5.57	41173/		
TQJC3H6OH<=>TQC3H5OHI		1.420E+036	-15.840		11594.0	
PLOG/	0.001	9.57E+58	-15.99	38293/		
PLOG/	0.01	7.27E+54	-14.25	38593/		
PLOG/	0.1	8.30E+49	-12.44	38031/		
PLOG/	1	1.90E+44	-10.51	36905/		
PLOG/	10	2.18E+36	-7.9	34865/		
PLOG/	40	4.10E+31	-6.36	33581/		
PLOG/	100	3.00E+28	-5.35	32704/		
PLOG/	200	1.34E+26	-4.59	32035/		
TQC3H6OI<=>CH3CHO+CH2O+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	8.09E+38	-9.91	19096/		
PLOG/	0.01	9.09E+39	-9.93	19135/		

PLOG/	0.1	1.89E+41	-10.02	19407/		
PLOG/	1	7.47E+23	-4.1	14658/		
PLOG/	10	2.95E+33	-6.75	18685/		
PLOG/	40	4.24E+36	-7.56	20307/		
PLOG/	100	7.83E+36	-7.54	20747/		
PLOG/	200	7.63E+35	-7.17	20641/		
QC3H5OHP<=>C3H5OH+HO2		1.420E+036	-15.840	11594.0		
PLOG/	0.001	3.29E+57	-15.64	28576/		
PLOG/	0.01	9.65E+58	-15.75	29927/		
PLOG/	0.1	2.19E+50	-12.66	28547/		
PLOG/	1	1.67E+49	-12.05	29204/		
PLOG/	10	7.08E+40	-9.26	27188/		
PLOG/	40	1.32E+30	-5.82	24071/		
PLOG/	100	1.15E+30	-5.8	24053/		
PLOG/	200	1.12E+30	-5.8	24050/		
QC3H5OHP<=>CY (COC) COH+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.11E+51	-12.97	28497/		
PLOG/	0.01	5.58E+51	-12.87	29529/		
PLOG/	0.1	3.03E+44	-10.28	28326/		
PLOG/	1	1.42E+44	-9.98	28986/		
PLOG/	10	9.69E+37	-7.93	27491/		
PLOG/	40	5.90E+29	-5.3	25095/		
PLOG/	100	5.27E+29	-5.29	25081/		
PLOG/	200	5.15E+29	-5.28	25078/		
TQC3H5OHI<=>CCY (COC) OH+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.10E+31	-7.21	14640/		
PLOG/	0.01	1.37E+32	-7.24	14716/		
PLOG/	0.1	3.34E+33	-7.35	15127/		
PLOG/	1	1.86E+23	-3.68	12864/		
PLOG/	10	9.88E+31	-6.23	16040/		
PLOG/	40	1.25E+34	-6.78	17056/		
PLOG/	100	7.73E+33	-6.67	17176/		
PLOG/	200	2.13E+33	-6.45	17170/		
TQC3H5OHI<=>SC3H5OH+HO2		1.420E+036	-15.840	11594.0		
PLOG/	0.001	6.01E+27	-7.27	14658/		
PLOG/	0.01	7.78E+28	-7.3	14733/		
PLOG/	0.1	3.27E+30	-7.48	15191/		
PLOG/	1	2.81E+17	-2.82	12336/		
PLOG/	10	1.92E+26	-5.22	16146/		
PLOG/	40	7.61E+27	-5.49	17483/		
PLOG/	100	1.91E+26	-4.86	17429/		
PLOG/	200	2.94E+24	-4.18	17285/		
C3H6OH2-1+O2<=>IQJC3H6OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	3.34+111	-32.67	25143/		
PLOG/	0.01	4.84+107	-31.05	25460/		
PLOG/	0.1	2.41+100	-28.42	24474/		
PLOG/	1	4.55E+89	-24.78	22176/		
PLOG/	10	1.14E+76	-20.31	18721/		
PLOG/	40	9.25E+66	-17.35	16238/		
PLOG/	100	6.20E+60	-15.36	14499/		
PLOG/	200	1.30E+56	-13.86	13159/		
C3H6OH2-1+O2<=>IC2H4OHCHO+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.59E+15	-1.63	8947/		
PLOG/	0.01	5.07E+20	-3.24	11938/		
PLOG/	0.1	5.00E+25	-4.66	15251/		
PLOG/	1	3.18E+26	-4.79	17388/		

PLOG/	10	6.00E+20	-2.95	17297/
PLOG/	40	1.70E+14	-0.91	16099/
PLOG/	100	7.91E+08	0.73	14913/
PLOG/	200	3.03E+04	2.08	13854/

C3H6OH2-1+O2<=>IQC3H6OT		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.12+102	-32.4	23496/
PLOG/	0.01	4.23E+95	-30.04	22067/
PLOG/	0.1	3.45E+83	-26.08	17114/
PLOG/	1	8.16E+82	-25.61	16198/
PLOG/	10	1.04E+97	-29.54	22648/
PLOG/	40	7.25+103	-31.42	26487/
PLOG/	100	2.48+106	-32.06	28397/
PLOG/	200	1.39+107	-32.2	29446/

C3H6OH2-1+O2<=>CH3CHO+CH2O+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	4.39E+48	-11.88	11603/
PLOG/	0.01	9.82E+50	-12.49	14143/
PLOG/	0.1	3.43E+49	-11.94	15561/
PLOG/	1	2.43E+45	-10.56	16415/
PLOG/	10	4.98E+39	-8.68	17473/
PLOG/	40	7.99E+33	-6.83	17502/
PLOG/	100	1.02E+29	-5.28	17165/
PLOG/	200	7.18E+24	-3.99	16747/

C3H6OH2-1+O2<=>CH3+CHOCH2OOH		1.420E+036	-15.840	11594.0
PLOG/	0.001	2.91E+40	-9.23	10830/
PLOG/	0.01	9.66E+43	-10.2	13698/
PLOG/	0.1	1.34E+44	-10.13	15661/
PLOG/	1	2.57E+41	-9.18	17047/
PLOG/	10	1.82E+36	-7.46	18330/
PLOG/	40	8.82E+29	-5.44	18205/
PLOG/	100	1.74E+24	-3.65	17600/
PLOG/	200	2.16E+19	-2.12	16925/

C3H6OH2-1+O2<=>IQC3H5OHPJ		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.03+115	-35.13	25407/
PLOG/	0.01	1.10+129	-38.89	32891/
PLOG/	0.1	5.15+135	-40.38	38573/
PLOG/	1	7.27+129	-38.13	39933/
PLOG/	10	4.50+112	-32.49	37045/
PLOG/	40	7.72E+97	-27.79	33612/
PLOG/	100	5.17E+86	-24.26	30799/
PLOG/	200	4.70E+77	-21.41	28440/

C3H6OH2-1+O2<=>C2H3OH+CH2O+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	5.10E+24	-4.31	13009/
PLOG/	0.01	6.91E+33	-6.97	17935/
PLOG/	0.1	1.74E+41	-9.03	23613/
PLOG/	1	2.26E+36	-7.32	25633/
PLOG/	10	3.15E+17	-1.4	22782/
PLOG/	40	9.35E+00	3.71	19114/
PLOG/	100	5.59E-12	7.46	16156/
PLOG/	200	1.27E-21	10.41	13733/

C3H6OH2-1+O2<=>CY(CCOC)OH+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	3.06E+33	-7.24	11476/
PLOG/	0.01	6.56E+42	-9.92	17197/

PLOG/	0.1	8.24E+46	-10.95	22090/	
PLOG/	1	4.48E+38	-8.22	23019/	
PLOG/	10	1.01E+18	-1.77	19496/	
PLOG/	40	1.16E+01	3.44	15637/	
PLOG/	100	4.85E-12	7.23	12599/	
PLOG/	200	8.64E-22	10.21	10126/	
!					
IQJC3H6OH<=>CHOCOHCH3+OH		1.420E+036	-15.840	11594.0	
PLOG/	0.001	3.58E+71	-20.62	52656/	
PLOG/	0.01	9.67E+71	-20.08	54935/	
PLOG/	0.1	3.39E+67	-18.18	55330/	
PLOG/	1	7.26E+58	-15.09	54016/	
PLOG/	10	4.57E+46	-11.01	51172/	
PLOG/	40	4.31E+38	-8.38	49054/	
PLOG/	100	2.12E+33	-6.66	47587/	
PLOG/	200	2.72E+29	-5.41	46486/	
!					
IQJC3H6OH<=>IQC3H6OT		1.420E+036	-15.840	11594.0	
PLOG/	0.001	1.04E+45	-11.2	31755/	
PLOG/	0.01	2.90E+40	-9.62	30945/	
PLOG/	0.1	4.85E+35	-8.01	29850/	
PLOG/	1	2.62E+30	-6.28	28498/	
PLOG/	10	3.37E+24	-4.37	26873/	
PLOG/	40	9.75E+20	-3.23	25861/	
PLOG/	100	5.61E+18	-2.52	25208/	
PLOG/	200	1.44E+17	-2.01	24740/	
IQJC3H6OH<=>IQC3H5OHPJ		1.420E+036	-15.840	11594.0	
PLOG/	0.001	1.36E+50	-12.93	36743/	
PLOG/	0.01	3.36E+45	-11.27	36143/	
PLOG/	0.1	1.13E+40	-9.41	34990/	
PLOG/	1	5.93E+33	-7.33	33438/	
PLOG/	10	4.24E+26	-5	31502/	
PLOG/	40	1.97E+22	-3.61	30275/	
PLOG/	100	3.43E+19	-2.72	29477/	
PLOG/	200	3.69E+17	-2.09	28900/	
IQC3H6OT<=>CH3CHO+CH2O+OH		1.420E+036	-15.840	11594.0	
PLOG/	0.001	9.82E+39	-9.95	20737/	
PLOG/	0.01	1.19E+41	-9.97	20814/	
PLOG/	0.1	2.60E+42	-10.07	21229/	
PLOG/	1	2.63E+32	-6.47	19139/	
PLOG/	10	1.32E+40	-8.68	22120/	
PLOG/	40	4.04E+41	-9.03	23000/	
PLOG/	100	9.07E+40	-8.77	23008/	
PLOG/	200	6.70E+39	-8.38	22782/	
IQC3H6OT<=>CH3+CHOCH2OOH		1.420E+036	-15.840	11594.0	
PLOG/	0.001	2.04E+37	-9.27	20741/	
PLOG/	0.01	2.54E+38	-9.29	20821/	
PLOG/	0.1	7.13E+39	-9.42	21267/	
PLOG/	1	2.95E+28	-5.34	18891/	
PLOG/	10	1.31E+36	-7.46	22106/	
PLOG/	40	2.19E+37	-7.68	23084/	
PLOG/	100	1.39E+36	-7.22	23018/	
PLOG/	200	2.67E+34	-6.63	22672/	
IQC3H5OHPJ<=>C2H3OH+CH2O+OH		1.420E+036	-15.840	11594.0	

PLOG/	0.001	4.25E+16	-3.66	19364/
PLOG/	0.01	2.98E+33	-8.01	27106/
PLOG/	0.1	3.46E+38	-8.83	31412/
PLOG/	1	7.07E+28	-5.46	29633/
PLOG/	10	2.01E+13	-0.43	25278/
PLOG/	40	1.43E+13	-0.38	25238/
PLOG/	100	1.38E+13	-0.38	25234/
PLOG/	200	1.37E+13	-0.37	25233/

IQC3H5OHPJ<=>CY (CCOC) OH+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.12E+25	-5.59	19349/
PLOG/	0.01	7.20E+32	-7.6	23093/
PLOG/	0.1	2.22E+34	-7.65	25130/
PLOG/	1	2.40E+27	-5.28	23663/
PLOG/	10	2.24E+17	-2.04	20810/
PLOG/	40	1.82E+17	-2.01	20786/
PLOG/	100	1.78E+17	-2.01	20783/
PLOG/	200	1.77E+17	-2.01	20782/

IQC3H5OHPJ<=>AC3H5OOH+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	6.07E+13	-4.21	22478/
PLOG/	0.01	9.74E+39	-10.89	33616/
PLOG/	0.1	2.18E+49	-12.65	40359/
PLOG/	1	3.32E+37	-8.42	38539/
PLOG/	10	2.34E+16	-1.56	32712/
PLOG/	40	1.44E+16	-1.49	32656/
PLOG/	100	1.38E+16	-1.48	32651/
PLOG/	200	1.37E+16	-1.48	32649/

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IQC4H7OHT<=>CH2COHCH2OOH+CH3		4.95E+10	0.83	27900
IQC4H8OT<=>CH3COCH3+CH2O+OH		3.64E+09	1.3	23700.0
IQC4H8OT<=>CH3+CH3COCO		4.95E+10	0.83	27900

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!C3H6OH1-2+O2<=>CCY (COC) OH+OH		1.420E+036	-15.840	11594.0
!PLOG/	0.001	2.84E+31	-6.95	6210/
!PLOG/	0.01	1.04E+36	-8.24	9233/
!PLOG/	0.1	1.15E+38	-8.76	11715/
!PLOG/	1	5.72E+35	-7.95	12823/
!PLOG/	10	2.74E+31	-6.51	13646/
!PLOG/	40	4.30E+28	-5.56	14541/
!PLOG/	100	2.40E+25	-4.51	14778/
!PLOG/	200	6.62E+21	-3.37	14606/

!

!TQC3H5OHI<=>CCY (COC) OH+OH		1.420E+036	-15.840	11594.0
!PLOG/	0.001	2.20E+30	-7.21	14640/
!PLOG/	0.01	2.74E+31	-7.24	14716/
!PLOG/	0.1	6.68E+32	-7.35	15127/
!PLOG/	1	3.72E+22	-3.68	12864/
!PLOG/	10	1.98E+31	-6.23	16040/
!PLOG/	40	2.50E+33	-6.78	17056/
!PLOG/	100	1.55E+33	-6.67	17176/
!PLOG/	200	4.26E+32	-6.45	17170/

!

!

!!MULTIPLY BY 2.0

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!TQJC3H6OH<=>TQC3H5OHI      1.420E+036   -15.840   11594.0
!PLOG/   0.001      1.91E+59-15.99   38293/
!PLOG/   0.01      1.45E+55-14.25   38593/
!PLOG/   0.1      1.66E+50-12.44   38031/
!PLOG/    1      3.80E+44-10.51   36905/
!PLOG/   10      4.36E+36-7.9   34865/
!PLOG/   40      8.20E+31-6.36 33581/
!PLOG/  100      6.00E+28-5.35 32704/
!PLOG/  200      2.68E+26-4.59 32035/
!
! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, COMBUST AND FLAME, 2011, 158,
726-731
CY(COC) COH+OH=>C2H2OH+CH2O+H2O      1.26E3      2.97      -2660.6

! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, IJCK, 2012, 44, 155-164
CY(COC) COH+HO2=>C2H2OH+CH2O+H2O2     1.4E-5      5.26      8267.9

! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233
CY(COC) COH+OH=>C2H3CHO+OH+H2O      5.66E2      2.93      -4039.4
CY(COC) COH+OH=>CH2CO+CH2OH+H2O     2.26E3      2.73      -4688
CCY(COC) OH+OH=>CH3CHCO+OH+H2O      2.26E3      2.73      -4688
CY(CCOC) OH+OH=>CH2O+C2H2OH+H2O     5.66E2      2.93      -4039.4
CY(CCOC) OH+OH=>CH2O+CH2CO+H+H2O    2.26E3      2.73      -4688

! J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308
CY(COC) COH+HO2=>C2H3CHO+OH+H2O     1.81E-1      3.98      9056.7
CY(COC) COH+HO2=>CH2CO+CH2OH+H2O2    8.6         3.46      9732.326
CCY(COC) OH+HO2=>CH3CHCO+OH+H2O     8.6         3.46      9732.326
CY(CCOC) OH+HO2=>CH2O+C2H2OH+H2O     1.81E-1      3.98      9056.7
CY(CCOC) OH+HO2=>CH2O+CH2CO+H+H2O    8.6         3.46      9732.326

!REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
CHOCOHC3+OH=>CH3CHCO+OH+H2O      61329.9     2.65     -4586.4

! C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION
! ANALOGY TO O2 + QOOH_2
TQC3H5OHI+O2<=>TQC3H5OHIO2      5.05E+12     -0.1      -
695.45
TQC3H5OHIO2<=>TQC3H5OHIO2-I      2.56E+12     -0.13     34360
TQC3H5OHIO2-I<=>HO2CHO+CH3CHO+OH   5.819E+05    2.40     22790
TQC3H5OHIO2-I<=>C3KET12+HO2       1.829E+10    0.790    15100
C3KET12=>CH3CHO+HCO+OH           9.500E+015   0.000    42540.0
TQC3H5OHIO2<=>TQC3H5OHIO2-P      5.69E+08     7.80E-01
21850
TQC3H5OHIO2-P<=>C2H3COHOOH+HO2    1.83E+10     7.90E-01
15100
TQC3H5OHIO2-P<=>C2H3OOH+HOCHO+OH   5.38E+11     0.070    24800
TQC3H5OHIO2-P<=>COHOHCY(COC)+OH   2.28E+08     1.29E+00
9890
TQC3H5OHIO2-P<=>OHCY(COCC)OOH+OH   4.58E+15     -1.08E+00
18440
C2H3COHOOH=>HOCHO+C2H3+OH        1.59E+20     -1.5
42879.46
C2H3OOH=>CH2CO+H+OH              1.59E+20     -1.5
42879.46

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COHOOHCY (COC) =>HOCHO+CH2CHO+OH 42879.46	1.59E+20	-1.5	
OHCY (COCC) OOH=>HOCHO+CH2CHO+OH 42879.46	1.59E+20	-1.5	
TQC3H5OHIO2<=>TQC3H5OHTO2	2.956E+09	0.04	16350
TQC3H5OHTO2<=>OHCOCOHHCH3+OH	1.2E+10	0.35	15700
OHCOCOHHCH3=>CO+CH3CHO+2OH 42879.46	1.59E+20	-1.5	
IQC3H5OHPJ+O2<=>IQC3H5OHPJO2	9.35626E+11	0.1	-1072.98
IQC3H5OHPJO2<=>IQC3H5OTQ-I	4.13E+07	1.0	21070
IQC3H5OTQ-I=>OH+CH2O+CHOCH2OOH 15700	1.20E+10	0.35	
CHOCH2OOH=>OH+CH2O+HCO 42879.46	1.59E+20	-1.5	
IQC3H5OHPJO2<=>IQC3H5OHQ-SJ	8.204E10	0.13	19470
IQC3H5OHQ-SJ<=>CHOCOHHCH2OOH+OH	1.2E+10	0.35	15700
CHOCOHHCH2OOH=>OH+CH2O+H+CHOCHO 42879.46	1.59E+20	-1.5	
CHOCHO+OH=>HCO+CO+H2O	61329.9	2.65	-4586.4

!!!!!!!!!!!!!!!!!!!!!!!!!!!!END OF FIRST & SECOND O2 ADDITION
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!REF:BILL SEPT 2013

!REF:FOR SC3H5OH, ASSUME THAT THE ALLYL HYDROGEN IS ABSTRACTED AND THEN C2H3CHO+H ARE FORMED.

!REF: USE RATE PRIMARY ALLYLIC

!REF: USED RATE OF C3H6+R<=>C2H5-A+RH.

!REF: SAUDI ARAMCO MECH 1.3 (NO REFERENCE)

SC3H5OH+O2=>C2H3CHO+H+HO2 39100.0	3.000E+013	0.000	
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!REF: TSANG 1991

SC3H5OH+OH=>C2H3CHO+H+H2O -298.0	3.100E+006	2.000	
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SC3H5OH+H=>C2H3CHO+H+H2 2492.0	1.730E+005	2.500	
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SC3H5OH+O=>C2H3CHO+H+OH 5884.0	1.750E+012	0.700	
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SC3H5OH+HO2=>C2H3CHO+H+H2O2 13900.0	9.600E+003	2.600	
----------------------------------------	------------	-------	--

SC3H5OH+CH3=>C2H3CHO+H+CH4 5675.0	2.210E+000	3.500	
--------------------------------------	------------	-------	--

!REF: USE HO2 ABSTRACTION RATE CONSTANT

SC3H5OH+CH3O2=>C2H3CHO+H+CH3O2H 13900.0	9.600E+003	2.600	
--------------------------------------------	------------	-------	--

!REF: USED SECONDARY ALKYL H RATE FOR N-ALKANE+CH3O,

!REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONARY ALKYL AND PRIMARY ALLYLIC WITH F<=>.2: 0.2(98.4-88.2)<=>.2*10.2<=>2.0

!REF: EST. F IS LARGER THAN OH WHICH IS 0.1. REDUCED A FACTOR BY 2.6 FOR TYING UP ROTOR (USED SCOTT AND WALKERS, C&F2002 A-FACTORS TO GET 2.6)
SC3H5OH+CH3O=>C2H3CHO+H+CH3OH 8.300E+010 0.000
2600.0

!REF: FROM PROPANOL, MAN ET AL. CNF2013:

!REF: !DASILVA, BOZZELLI, CHEM. PHYS. LETT. 483 (2009) 25-29.
SC3H5OH+HO2<=>C2H5CHO+HO2 1.490E+005 1.670
6810.0

!REF: !DASILVA, ANGEW. CHEM. 122 (2010) 7685-7687
SC3H5OH+HOCHO<=>C2H5CHO+HOCHO 2.810E-002 3.286
-4509.0

!REF: SARATHY ET AL. CNF2012
SC3H5OH<=>C2H5CHO 8.590E+011 0.318
55900.0

!REF: WILK, CERNANSKY, PITZ, AND WESTBROOK, C&F 1988.
C3H6OH1-2+O2<=>HOC3H6O2 1.200E+011 0.000
-1100.0

!REF:
HOC3H6O2=>CH3CHO+CH2O+OH 1.250E+010 0.000
18900.0

!REF: DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
C2H2+CH3<=>C3H5-A 8.200E+053 -13.320
33200.0

PLOG/	0.1000	8.200E+053	-13.320	33200.0/
PLOG/	1.0000	2.680E+053	-12.820	35730.0/
PLOG/	2.0000	3.640E+052	-12.460	36127.0/
PLOG/	5.0000	1.040E+051	-11.890	36476.0/
PLOG/	10.0000	4.400E+049	-11.400	36700.0/
PLOG/	100.0000	3.800E+044	-9.630	37600.0/

!REF: ANOLOGY WITH C3H5-A+HO2
C3H5-A+CH3O2<=>C3H5O+CH3O 1.000E+011 0.000
0.0

PLOG/	0.0100	3.330E+012	-0.158	-1417.0/
PLOG/	0.1000	1.660E+014	-0.642	-349.1/
PLOG/	1.0000	2.595E+017	-1.520	2379.2/
PLOG/	10.0000	9.780E+014	-0.684	3615.3/
PLOG/	100.0000	5.470E+003	2.740	1144.4/

C3H5-A+CH3O2<=>AC4H7OOH 1.000E+011 0.000
0.0

PLOG/	0.0100	1.910E+031	-7.230	1336.2/
PLOG/	0.1000	6.310E+042	-10.300	5568.9/
PLOG/	1.0000	1.030E+045	-10.600	7851.5/
PLOG/	10.0000	2.790E+037	-7.920	6497.9/
PLOG/	100.0000	3.400E+029	-5.280	4539.8/

AC4H7OOH<=>C3H5O+CH3O 1.000E+011 0.000
0.0

PLOG/	0.0100	1.490E+058	-13.900	54266.9/	
PLOG/	0.1000	1.800E+054	-12.400	54193.8/	
PLOG/	1.0000	3.360E+046	-9.810	52468.5/	
PLOG/	10.0000	2.390E+036	-6.540	49429.0/	
PLOG/	100.0000	2.560E+027	-3.610	46333.1/	
!REF:KLIPPENSTEIN & HARDING 2007					
C3H5-A+H<=>C3H4-A+H2				1.232E+003	3.035
2582.0					
!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.					
C3H5-A+O<=>C2H3CHO+H				6.000E+013	0.000
0.0					
!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.					
C3H5-A+OH=>C2H3CHO+H+H				5.300E+037	-6.710
29306.0					
PLOG/	0.1000	5.300E+037	-6.710	29306.0/	
PLOG/	1.0000	4.200E+032	-5.160	30126.0/	
PLOG/	10.0000	1.600E+020	-1.560	26330.0/	
!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.					
C3H5-A+OH<=>C3H4-A+H2O				6.000E+012	0.000
0.0					
!REF:LASKIN ET AL. IJCK 32 589-614 2000					
C3H5-A+CH3<=>C3H4-A+CH4				3.000E+012	-0.320
-131.0					
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).					
C3H5-A+C2H5<=>C2H6+C3H4-A				4.000E+011	0.000
0.0					
C3H5-A+C2H5<=>C2H4+C3H6				4.000E+011	0.000
0.0					
C3H5-A+C2H3<=>C2H4+C3H4-A				1.000E+012	0.000
0.0					
!REF:!WANG, J. PHYS. CHEM. REF. DATA 20, 221-273, (1991)					
!REF:LASKIN ET AL. IJCK 32 589-614 2000					
C3H5-A+O2<=>C3H4-A+HO2				4.990E+015	-1.400
22428.0					
PLOG/	1.0000	4.990E+015	-1.400	22428.0/	
PLOG/	10.0000	2.180E+021	-2.850	30755.0/	
C3H5-A+O2<=>CH3CO+CH2O				1.190E+015	-1.010
20128.0					
PLOG/	1.0000	1.190E+015	-1.010	20128.0/	
PLOG/	10.0000	7.140E+015	-1.210	21046.0/	
C3H5-A+O2<=>C2H3CHO+OH				1.820E+013	-0.410
22859.0					
PLOG/	1.0000	1.820E+013	-0.410	22859.0/	
PLOG/	10.0000	2.470E+013	-0.450	23017.0/	
!REF:LASKIN ET AL. IJCK 32 589-614 2000					
C3H5-A+HCO<=>C3H6+CO				6.000E+013	0.000
0.0					
C2H3+CH3<=>C3H5-A+H				1.500E+024	-2.830
18618.0					

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 C3H5-A<=>C3H5-T 3.900E+059 -15.420
 75400.0
 PLOG/ 0.1000 3.900E+059 -15.420 75400.0/
 PLOG/ 1.0000 7.060E+056 -14.080 75868.0/
 PLOG/ 2.0000 4.800E+055 -13.590 75949.0/
 PLOG/ 5.0000 4.860E+053 -12.810 75883.0/
 PLOG/ 10.0000 6.400E+051 -12.120 75700.0/
 PLOG/ 100.0000 2.800E+043 -9.270 74000.0/

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 C3H5-A<=>C3H5-S 1.300E+055 -14.530
 73800.0
 PLOG/ 0.1000 1.300E+055 -14.530 73800.0/
 PLOG/ 1.0000 5.000E+051 -13.020 73300.0/
 PLOG/ 10.0000 9.700E+048 -11.730 73700.0/
 PLOG/ 100.0000 4.860E+044 -9.840 73400.0/

!REF: ANALOGY C2H3+O2 KLIPPENSTEIN
 C3H5-S+O2<=>CH3CHO+HCO 3.100E+031 -5.944
 5748.4
 C3H5-S+O2<=>CH3CHCHO+O 5.380E+018 -2.140
 5142.9
 C3H5-S+O2<=>C2H3CHO+OH 2.700E+019 -2.140
 5142.9

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H5-S+H<=>C3H4-A+H2 3.333E+012 0.000
 0.0
 C3H5-S+CH3<=>C3H4-A+CH4 1.000E+011 0.000
 0.0

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 C2H2+CH3<=>C3H5-T 6.800E+020 -4.160
 18000.0
 PLOG/ 0.1000 6.800E+020 -4.160 18000.0/
 PLOG/ 1.0000 4.990E+022 -4.390 18850.0/
 PLOG/ 2.0000 6.000E+023 -4.600 19571.0/
 PLOG/ 5.0000 7.310E+025 -5.060 21150.0/
 PLOG/ 10.0000 9.300E+027 -5.550 22900.0/
 PLOG/ 100.0000 3.800E+036 -7.580 31300.0/

!REF:LASKIN ET AL. IJCK 32 589-614 2000
 C3H5-S+H<=>C3H4-P+H2 3.340E+012 0.000
 0.0
 C3H5-S+O<=>C2H4+HCO 6.000E+013 0.000
 0.0
 C3H5-S+OH=>C2H4+HCO+H 5.000E+012 0.000
 0.0
 C3H5-S+HO2=>C2H4+HCO+OH 2.000E+013 0.000
 0.0
 C3H5-S+HCO<=>C3H6+CO 9.000E+013 0.000
 0.0
 C3H5-S+CH3<=>C3H4-P+CH4 1.000E+011 0.000
 0.0

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 C3H5-T<=>C3H5-S 1.600E+044 -12.160
 52200.0
 PLOG/ 0.1000 1.600E+044 -12.160 52200.0/
 PLOG/ 1.0000 1.500E+048 -12.710 53900.0/
 PLOG/ 10.0000 5.100E+052 -13.370 57200.0/
 PLOG/ 100.0000 5.800E+051 -12.430 59200.0/

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 C3H4-A+H<=>C3H5-S 1.100E+030 -6.520
 15200.0
 PLOG/ 0.1000 1.100E+030 -6.520 15200.0/
 PLOG/ 1.0000 5.400E+029 -6.090 16300.0/
 PLOG/ 10.0000 2.600E+031 -6.230 18700.0/
 PLOG/ 100.0000 3.200E+031 -5.880 21500.0/

!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)
 C3H4-A+C3H4-A<=>C3H5-A+C3H3 5.000E+014 0.000
 64746.7

!REF:LASKIN ET AL. IJCK 32 589-614 2000
 C3H5-T+O2<=>CH3COCH2+O 9.860E+025 -3.751
 11255.4
 C3H5-T+O2<=>CH3CO+CH2O 2.550E+020 -2.608
 1565.7
 C3H5-T+O2<=>C3H4-A+HO2 3.590E+010 -0.270
 -413.6

!!REF:LASKIN ET AL. IJCK 32 589-614 2000 ANALOGY WITH C2H3+O2
 !C3H5-T+O2<=>CH3COCH2+O 1.24E+13 -0.12
 1696
 !C3H5-T+O2<=>CH3CO+CH2O 8.60E+21 -2.97
 3320
 !C3H5-T+O2<=>C3H4-A+HO2 1.00E+11 0 0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
 C3H5-T+H<=>C3H4-P+H2 3.340E+012 0.000
 0.0
 C3H5-T+CH3<=>C3H4-P+CH4 1.000E+011 0.000
 0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
 C3H5-T+O<=>CH3+CH2CO 6.000E+013 0.000
 0.0
 C3H5-T+OH=>CH3+CH2CO+H 5.000E+012 0.000
 0.0
 C3H5-T+HO2=>CH3+CH2CO+OH 2.000E+013 0.000
 0.0
 C3H5-T+HCO<=>C3H6+CO 9.000E+013 0.000
 0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H4-A+HO2=>CH2CO+CH2+OH 4.000E+012 0.000
 19000.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-A+O<=>C2H4+CO 1000.0	2.000E+007	1.800
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-A+O<=>C2H2+CH2O -4243.0	3.000E-003	4.610
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-A+CH3<=>C3H3+CH4 7700.0	1.300E+012	0.000
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-A+C3H5-A<=>C3H3+C3H6 7700.0	2.000E+011	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-A+C2H<=>C2H2+C3H3 0.0	1.000E+013	0.000
!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 C3H4-P+H<=>C3H5-A 28100.0	1.100E+060	-14.560
PLOG/ 0.1000	1.100E+060	-14.560
PLOG/ 1.0000	4.910E+060	-14.370
PLOG/ 2.0000	3.040E+060	-14.190
PLOG/ 5.0000	9.020E+059	-13.890
PLOG/ 10.0000	2.200E+059	-13.610
PLOG/ 100.0000	1.600E+055	-12.070
28100.0/		
31644.0/		
32642.0/		
33953.0/		
34900.0/		
37500.0/		
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-P+C3H3<=>C3H4-A+C3H3 10450.0	6.140E+006	1.740
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-P+O<=>HCCO+CH3 2250.0	7.300E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-P+O<=>C2H4+CO 2250.0	1.000E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-P+C2H<=>C2H2+C3H3 0.0	1.000E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H4-P+CH3<=>C3H3+CH4 7700.0	1.800E+012	0.000
!REF:PITZ ESTIMATE C2H+CH3<=>C3H4-P 0.0	8.000E+013	0.000

!REF:LASKIN ET AL. IJCK 32 589-614 2000		
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-P+HO2=>C2H4+CO+OH 19000.0	3.000E+012	0.000
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-P+O<=>C2H3+HCO 2010.0	3.200E+012	0.000
!REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST C3H4-P+O<=>C3H3+OH 8600.0	7.650E+008	1.500
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-P+C2H3<=>C3H3+C2H4 7700.0	1.000E+012	0.000
!C3H4-P+C3H5-A<=>C3H3+C3H6 7700.0	3.000E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H3+O<=>CH2O+C2H 0.0	2.000E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H3+HO2=>OH+CO+C2H3 0.0	8.000E+011	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H3+HCO<=>C3H4-A+CO 0.0	2.500E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000 C3H3+HCO<=>C3H4-P+CO 0.0	2.500E+013	0.000
!REF: C2H5+C2H<=>C3H3+CH3 0.0	1.810E+013	0.000
!REF:DAGAUT, P. ET AL., CST 71, 111(1990). C3H4-A+HO2=>C2H4+CO+OH 14000.0	1.000E+011	0.000
C3H4-A+HO2<=>C3H3+H2O2 9632.8	3.580E-002	4.170
C3H4-A+CH3O2<=>C3H3+CH3O2H 9632.8	7.161E-002	4.170
C3H4-P+HO2<=>C3H3+H2O2 9632.8	9.550E-002	4.170
C3H4-P+CH3O2<=>C3H3+CH3O2H 9632.8	9.550E-002	4.170
!REF: ESTIMATE ATKINSON 1984 C3 NUIG S.M.B C3H4-A+OH<=>CH2CCH2OH -304.0	1.110E+012	0.000

C3H4-A+OH<=>SC3H4OH 2.220E+012 0.000
-304.0

!REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP

CH2CCH2OH<=>CH2O+C2H3 9.240E+010 0.870
30460.0

CH2CCH2OH<=>C2H3CHO+H 1.110E+011 0.480
36770.0

CH2CCH2OH<=>HCO+C2H4 9.240E+010 0.870
30460.0

SC3H4OH<=>CH2CO+CH3 9.240E+010 0.870
30460.0

C3H4-A+H<=>C3H3+H2 6.625E+003 3.095
5522.0

!REF: ANALOGIES WITH C3H6 A AND S

C3H4-P+OH<=>C3H3+H2O 4.940E+006 2.027
1059.6

C3H4-A+OH<=>C3H3+H2O 1.482E+005 2.492
1807.2

C3H4-P+H<=>C3H3+H2 3.572E+004 2.825
4821.0

!REF: ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984

C3H4-P+OH<=>PC3H4OH-2 3.930E+011 0.000
0.0

C3H4-P+OH<=>SC3H4OH 2.360E+012 0.000
0.0

!REF: MATHEU ET AL. IJCK, 2003, 35, 95--119

PC3H4OH-2<=>CH3CHCHO 3.560E+010 0.880
23238.0

!REF: PELUCCHI ECM 2013

CH3CHCHO<=>C2H3CHO+H 4.164E+012 -0.020
32410.0

CH3CHCHO<=>CH3CHCO+H 8.328E+012 -0.020
32410.0

C3H3+H<=>C3H2+H2 2.140E+005 2.520
7453.0

C3H3+H<=>C3H2 (S) +H2 3.311E+013 0.195
17579.0

PLOG/ 0.0395 2.951E+009 1.280 13474.0/
PLOG/ 1.0000 1.097E+010 1.130 13929.0/

PLOG/ 10.0000 3.311E+013 0.195 17579.0/
C3H3+H<=>H2CCC (S) +H2 1.000E+018 -1.230
15111.0

PLOG/ 0.0395 2.692E+009 1.050 5371.0/
PLOG/ 1.0000 2.884E+013 -0.030 9448.0/

PLOG/ 10.0000 1.000E+018 -1.230 15111.0/
C3H3+H<=>C3H2C+H2 7.244E+009 0.606
18356.0

PLOG/ 0.0395 1.072E+007 1.370 15557.0/
PLOG/ 1.0000 1.349E+007 1.340 15560.0/

PLOG/ 10.0000 7.244E+009 0.606 18356.0/
C3H4-A<=>C3H4-P 4.786E+048 -10.000
88685.0

PLOG/ 1.0000 7.762E+039 -7.800 78446.0/

PLOG/	10.0000	4.786E+048	-10.000	88685.0/	
CC3H4<=>C3H4-P				1.660E+037	-7.240
48013.0					
PLOG/	0.0395	2.512E+050	-11.820	50914.0/	
PLOG/	1.0000	1.230E+037	-7.510	45551.0/	
PLOG/	10.0000	1.660E+037	-7.240	48013.0/	
CC3H4<=>C3H4-A				5.012E+035	-6.870
51298.0					
PLOG/	0.0395	9.772E+043	-9.970	56007.0/	
PLOG/	1.0000	2.512E+026	-4.560	43922.0/	
PLOG/	10.0000	5.012E+035	-6.870	51298.0/	
C3H4-P<=>C3H3+H				6.480E+030	-4.655
93925.2					
PLOG/	1.0000	6.480E+030	-4.655	93925.2/	
PLOG/	10.0000	1.210E+025	-2.787	92376.1/	
C3H4-A<=>C3H3+H				1.320E+031	-4.749
92079.5					
PLOG/	1.0000	1.320E+031	-4.749	92079.5/	
PLOG/	10.0000	3.650E+025	-2.950	90624.9/	
C3H3+H<=>CC3H4				3.236E+018	-2.050
2053.0					
PLOG/	0.0395	8.913E+112	-28.260	83611.0/	
PLOG/	1.0000	1.072E+021	-2.950	2687.0/	
PLOG/	10.0000	3.236E+018	-2.050	2053.0/	
C3H2 (S) +M<=>C3H2+M				1.000E+013	0.000
0.0					
H2CCC (S) +O2<=>CO2+C2H2				1.000E+013	0.000
0.0					
C3H2 (S) +H<=>H2CCC (S) +H				1.000E+013	0.000
0.0					
C3H2C+O2<=>C2H2+CO2				1.000E+013	0.000
0.0					
!REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438					
C3H4-A+H<=>C3H5-A				2.210E+061	-15.250
20076.0					
PLOG/	0.0010	2.210E+061	-15.250	20076.0/	
PLOG/	0.0390	1.240E+052	-12.020	17839.0/	
PLOG/	1.0000	4.670E+051	-11.450	21340.0/	
PLOG/	10.0000	3.750E+048	-10.270	22511.0/	
PLOG/	100.0000	4.230E+043	-8.610	22522.0/	
DUP					
C3H4-A+H<=>C3H5-A				2.210E+061	-15.250
20076.0					
PLOG/	0.0010	2.800E+038	-8.670	8035.0/	
PLOG/	0.0390	9.330E+036	-8.190	7462.0/	
PLOG/	1.0000	3.320E+030	-5.780	6913.0/	
PLOG/	10.0000	2.290E+026	-4.320	6163.0/	
PLOG/	100.0000	4.380E+021	-2.710	5187.0/	
DUP					
C3H4-A+H<=>C3H4-P+H				2.440E+010	1.040
2159.0					
PLOG/	0.0010	8.490E+010	0.890	2503.0/	
PLOG/	0.0390	1.480E+013	0.260	4103.0/	
PLOG/	1.0000	2.480E+015	-0.330	6436.0/	
PLOG/	10.0000	2.350E+025	-3.230	13165.0/	
PLOG/	100.0000	1.020E+024	-2.670	15552.0/	
DUP					

C3H4-A+H<=>C3H4-P+H				2.440E+010	1.040
2159.0					
PLOG/	10.0000	1.790E+007	1.980	4521.0/	
PLOG/	100.0000	4.630E+004	2.620	4466.0/	
DUP					
C3H4-A+H<=>CH3+C2H2				3.740E+001	3.350
57.8					
PLOG/	0.0010	1.230E+008	1.530	4737.0/	
PLOG/	0.0390	2.720E+009	1.200	6834.0/	
PLOG/	1.0000	1.260E+020	-1.830	15003.0/	
PLOG/	10.0000	1.680E+016	-0.600	14754.0/	
PLOG/	100.0000	1.370E+017	-0.790	17603.0/	
DUP					
C3H4-A+H<=>CH3+C2H2				3.740E+001	3.350
57.8					
PLOG/	1.0000	1.230E+004	2.680	6335.0/	
PLOG/	10.0000	3.310E+008	1.140	8886.0/	
PLOG/	100.0000	1.280E+006	1.710	9774.0/	
DUP					
C3H4-A+H<=>C3H5-T				6.440E+102	-27.510
51768.0					
PLOG/	0.0010	6.440E+102	-27.510	51768.0/	
PLOG/	0.0390	1.550E+053	-13.100	14472.0/	
PLOG/	1.0000	1.900E+053	-12.590	16726.0/	
PLOG/	10.0000	7.950E+051	-11.820	18286.0/	
PLOG/	100.0000	4.210E+052	-11.640	22262.0/	
DUP					
C3H4-A+H<=>C3H5-T				6.440E+102	-27.510
51768.0					
PLOG/	0.0010	1.100E+054	-14.290	10809.0/	
PLOG/	0.0390	9.880E+044	-11.210	8212.0/	
PLOG/	1.0000	2.810E+040	-9.420	7850.0/	
PLOG/	10.0000	2.600E+035	-7.570	7147.0/	
PLOG/	100.0000	9.880E+029	-5.530	6581.0/	
DUP					
C3H4-P+H<=>C3H5-T				8.850E+051	-13.040
12325.0					
PLOG/	0.0010	8.850E+051	-13.040	12325.0/	
PLOG/	0.0390	3.170E+052	-12.690	14226.0/	
PLOG/	1.0000	2.870E+053	-12.510	16853.0/	
PLOG/	10.0000	9.510E+051	-11.740	18331.0/	
PLOG/	100.0000	4.510E+052	-11.580	22207.0/	
DUP					
C3H4-P+H<=>C3H5-T				8.850E+051	-13.040
12325.0					
PLOG/	0.0010	1.970E+046	-11.910	7456.0/	
PLOG/	0.0390	2.590E+045	-11.230	8046.0/	
PLOG/	1.0000	6.930E+039	-9.110	7458.0/	
PLOG/	10.0000	6.800E+034	-7.290	6722.0/	
PLOG/	100.0000	5.650E+029	-5.390	6150.0/	
DUP					
C3H4-P+H<=>C3H5-S				3.380E+049	-12.750
14072.0					
PLOG/	0.0390	3.380E+049	-12.750	14072.0/	
PLOG/	1.0000	1.370E+051	-12.550	15428.0/	
PLOG/	10.0000	3.880E+050	-11.900	16915.0/	
PLOG/	100.0000	2.170E+049	-11.100	18746.0/	
DUP					

C3H4-P+H<=>C3H5-S				3.380E+049	-12.750
14072.0					
PLOG/	0.0010	1.490E+038	-10.110	7458.0/	
PLOG/	0.0390	2.980E+043	-11.430	8736.0/	
PLOG/	1.0000	5.750E+039	-9.510	8772.0/	
PLOG/	10.0000	4.330E+040	-9.600	9401.0/	
PLOG/	100.0000	3.440E+034	-7.360	8558.0/	
DUP					
C3H4-P+H<=>CH3+C2H2				2.120E+010	1.060
3945.0					
PLOG/	0.0010	2.440E+010	1.040	3980.0/	
PLOG/	0.0390	3.890E+010	0.989	4114.0/	
PLOG/	1.0000	3.460E+012	0.442	5463.0/	
PLOG/	10.0000	1.720E+014	-0.010	7134.0/	
PLOG/	100.0000	1.900E+015	-0.290	8306.0/	
CH3+C2H2<=>C3H5-S				1.780E+042	-10.400
13647.0					
PLOG/	0.0010	1.780E+042	-10.400	13647.0/	
PLOG/	0.0390	1.520E+044	-10.730	15256.0/	
PLOG/	1.0000	1.190E+044	-10.190	18728.0/	
PLOG/	10.0000	6.020E+043	-9.740	20561.0/	
PLOG/	100.0000	1.420E+042	-8.910	22235.0/	
DUP					
CH3+C2H2<=>C3H5-S				1.780E+042	-10.400
13647.0					
PLOG/	1.0000	8.490E+035	-8.430	12356.0/	
PLOG/	10.0000	3.040E+032	-7.010	12357.0/	
PLOG/	100.0000	1.690E+027	-5.070	11690.0/	
DUP					
C3H4-A+O2<=>C3H3+HO2				4.000E+013	0.000
41320.0					
C3H4-P+O2<=>C3H3+HO2				3.000E+013	0.000
42630.0					
C3H3+OH<=>C3H2+H2O				2.000E+013	0.000
8000.0					
C3H3+OH<=>CH2O+C2H2				2.000E+012	0.000
0.0					
C3H3+OH<=>C2H3+HCO				1.000E+013	0.000
0.0					
C3H3+OH<=>C2H4+CO				1.000E+013	0.000
0.0					
C3H3+OH<=>C3H2 (S) +H2O				1.000E+012	0.000
0.0					
C3H3+OH<=>H2CCC (S) +H2O				1.000E+012	0.000
0.0					
C3H3+O2<=>CH2CO+HCO				1.700E+005	1.700
1500.0					
!REF: ANALOGY WITH C3H5-A+HO2 !KINETICS FROM FRANKLIN C GOLDSMITH !J.					
PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
C3H3+HO2<=>C3H3O+OH				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.020E+013	-0.158	-1417.0/	
PLOG/	0.1000	4.980E+014	-0.642	-349.1/	
PLOG/	1.0000	7.770E+017	-1.520	2379.2/	
PLOG/	10.0000	2.930E+015	-0.684	3615.3/	
PLOG/	100.0000	1.640E+004	2.740	1144.4/	

C3H3+HO2<=>C3H3O2H				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.910E+031	-7.230	1336.2/	
PLOG/	0.1000	6.310E+042	-10.300	5568.9/	
PLOG/	1.0000	1.030E+045	-10.600	7851.5/	
PLOG/	10.0000	2.790E+037	-7.920	6497.9/	
PLOG/	100.0000	4.730E+025	-4.130	2923.8/	
C3H3+HO2<=>C2HCHO+H2O				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.090E+000	3.010	-3421.1/	
PLOG/	0.1000	6.350E+001	2.500	-2341.4/	
PLOG/	1.0000	6.050E+005	1.390	595.1/	
PLOG/	10.0000	3.100E+005	1.590	2677.6/	
PLOG/	100.0000	5.070E-005	4.590	927.5/	
C3H3O2H<=>C2HCHO+H2O				1.000E+011	0.000
0.0					
PLOG/	0.0100	1.990E+050	-12.700	53531.9/	
PLOG/	0.1000	4.720E+047	-11.500	54360.9/	
PLOG/	1.0000	1.500E+040	-8.840	53179.2/	
PLOG/	10.0000	2.540E+028	-5.000	49919.4/	
PLOG/	100.0000	1.480E+016	-1.120	45949.3/	
C2H+CH2O<=>C3H3O				1.000E+011	0.000
0.0					
PLOG/	0.0010	5.925E-004	2.609	-4297.3/	
PLOG/	0.0100	5.688E+006	-0.073	-1234.1/	
PLOG/	0.1000	5.390E+013	-1.803	1452.2/	
PLOG/	1.0000	8.733E+015	-2.074	2510.1/	
PLOG/	10.0000	5.305E+019	-2.943	4532.2/	
PLOG/	100.0000	3.779E+021	-3.163	6802.5/	
C2HCHO<=>C2H2+CO				2.510E+014	0.000
68000.0					
C2H+HCO<=>C2HCHO				1.000E+013	0.000
0.0					

!REF:ESTIMATE

CH3CHCO+OH<=>C2H5+CO2				1.730E+012	0.000
-1010.0					
CH3CHCO+OH<=>SC2H4OH+CO				2.000E+012	0.000
-1010.0					
CH3CHCO+H<=>C2H5+CO				4.400E+012	0.000
1459.0					
CH3CHCO+O<=>CH3CHO+CO				3.200E+012	0.000
-437.0					

!REF:

NC3H7+HO2<=>NC3H7O+OH				7.000E+012	0.000
-1000.0					
IC3H7+HO2<=>IC3H7O+OH				7.000E+012	0.000
-1000.0					
CH3O2+NC3H7<=>CH3O+NC3H7O				7.000E+012	0.000
-1000.0					
CH3O2+IC3H7<=>CH3O+IC3H7O				7.000E+012	0.000
-1000.0					

!REF:

!*****

!NC3H7+O2<=>NC3H7O2	4.520E+012	0.000
0.0 !CMT OUT, KWZ 0822		
!IC3H7+O2<=>IC3H7O2	7.540E+012	0.000
0.0		
NC3H7+O2<=>NC3H7O2 1.0E11 0.0 0.0	! ADD KWZ 0822,	
GOLDSMITH JPCA 2012, 116 (13), PP 3325		
PLOG/ 0.01 9.2E+008 0.405 -4398.65/		
PLOG/ 0.1 1.45E+014 -0.984 -1710.8/		
PLOG/ 1 2.09E+013 -0.499 -938.423/		
PLOG/ 10 1.15E+020 -2.42 2451.26/		
PLOG/ 100 2.07E+016 -1.3 803.419/		
IC3H7+O2<=>IC3H7O2 1.0E11 0.0 0.0		
PLOG/ 0.01 7.33E+005 1.33 -6345.64/		
PLOG/ 0.1 2.24E+011 -0.105 -3697.87/		
PLOG/ 1 1.54E+018 -2.02 -498.567/		
PLOG/ 10 6.74E+027 -4.85 3779.82/		
PLOG/ 100 1.67E+029 -5.15 5036.45/		
!*****		

!REF:ANALOGY TO CH2O+HO2		
NC3H7O2+CH2O<=>NC3H7O2H+HCO	5.600E+012	0.000
13600.0		
!REF:HALF OF CH2O+HO2		
NC3H7O2+CH3CHO<=>NC3H7O2H+CH3CO	2.800E+012	0.000
13600.0		
!REF:ANALOGY TO CH2O+HO2		
IC3H7O2+CH2O<=>IC3H7O2H+HCO	5.600E+012	0.000
13600.0		
!REF:HALF OF CH2O+HO2		
IC3H7O2+CH3CHO<=>IC3H7O2H+CH3CO	2.800E+012	0.000
13600.0		
!REF:		
NC3H7O2+HO2<=>NC3H7O2H+O2	1.750E+010	0.000
-3275.0		
IC3H7O2+HO2<=>IC3H7O2H+O2	1.750E+010	0.000
-3275.0		
!REF:ANALOGY TO C2H4+HO2		
C2H4+NC3H7O2<=>C2H3+NC3H7O2H	1.130E+013	0.000
30430.0		
C2H4+IC3H7O2<=>C2H3+IC3H7O2H	1.130E+013	0.000
30430.0		
!REF:ANALOGY TO CH3OH+HO2		
CH3OH+NC3H7O2<=>CH2OH+NC3H7O2H	6.300E+012	0.000
19360.0		
CH3OH+IC3H7O2<=>CH2OH+IC3H7O2H	6.300E+012	0.000
19360.0		
!REF:HALF OF CH2O+HO2		
C2H3CHO+NC3H7O2<=>C2H3CO+NC3H7O2H	2.800E+012	0.000
13600.0		

C2H3CHO+IC3H7O2<=>C2H3CO+IC3H7O2H 13600.0	2.800E+012	0.000
!REF:ANALOGY TO CH4+HO2		
CH4+NC3H7O2<=>CH3+NC3H7O2H 24640.0	1.120E+013	0.000
CH4+IC3H7O2<=>CH3+IC3H7O2H 24640.0	1.120E+013	0.000
!REF:		
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2 1860.0	1.400E+016	-1.610
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
H2+NC3H7O2<=>H+NC3H7O2H 26030.0	3.010E+013	0.000
H2+IC3H7O2<=>H+IC3H7O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC3H7O2+C2H6<=>IC3H7O2H+C2H5 20460.0	1.700E+013	0.000
NC3H7O2+C2H6<=>NC3H7O2H+C2H5 20460.0	1.700E+013	0.000
IC3H7O2+C2H5CHO<=>IC3H7O2H+C2H5CO 9500.0	2.000E+011	0.000
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO 9500.0	2.000E+011	0.000
!REF:		
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2 1860.0	1.400E+016	-1.610
NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2 1860.0	1.400E+016	-1.610
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2 1860.0	1.400E+016	-1.610
NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+IC3H7O2=>O2+IC3H7O+IC3H7O 1860.0	1.400E+016	-1.610
NC3H7O2+NC3H7O2=>O2+NC3H7O+NC3H7O 1860.0	1.400E+016	-1.610
IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+CH3<=>IC3H7O+CH3O -1000.0	7.000E+012	0.000
IC3H7O2+C2H5<=>IC3H7O+C2H5O -1000.0	7.000E+012	0.000
IC3H7O2+IC3H7<=>IC3H7O+IC3H7O -1000.0	7.000E+012	0.000
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O -1000.0	7.000E+012	0.000
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O -1000.0	7.000E+012	0.000
NC3H7O2+CH3<=>NC3H7O+CH3O -1000.0	7.000E+012	0.000

NC3H7O2+C2H5<=>NC3H7O+C2H5O -1000.0	7.000E+012	0.000
NC3H7O2+IC3H7<=>NC3H7O+IC3H7O -1000.0	7.000E+012	0.000
NC3H7O2+NC3H7<=>NC3H7O+NC3H7O -1000.0	7.000E+012	0.000
NC3H7O2+C3H5-A<=>NC3H7O+C3H5O -1000.0	7.000E+012	0.000
NC3H7O2H<=>NC3H7O+OH 42500.0	1.500E+016	0.000
!REF:PITZ ESTIMATE		
IC3H7O+OH<=>IC3H7O2H 0.0	1.000E+015	-0.800
!REF:		
C2H5+CH2O<=>NC3H7O 3496.0	1.000E+011	0.000
C2H5CHO+H<=>NC3H7O 6260.0	4.000E+012	0.000
CH3+CH3CHO<=>IC3H7O 9256.0	1.000E+011	0.000
CH3COCH3+H<=>IC3H7O 7270.0	2.000E+012	0.000
!REF:BALLA ET AL., CHEM. PHYSICS, 99, 323 (1985)		
IC3H7O+O2<=>CH3COCH3+HO2 390.0	9.090E+009	0.000
!REF:		
NC3H7O2<=>C3H6OOH1-2 26850.0	6.000E+011	0.000
NC3H7O2<=>C3H6OOH1-3 24400.0	1.125E+011	0.000
IC3H7O2<=>C3H6OOH2-1 29400.0	1.800E+012	0.000
!REF:BOZZELLI, J. AND DEAN, A, 1992		
IC3H7O2<=>C3H6OOH2-2 48880.0	1.230E+035	-6.960
!REF:		
C3H6OOH1-2<=>C3H6O1-2+OH 22000.0	6.000E+011	0.000
C3H6OOH1-3<=>C3H6O1-3+OH 15250.0	7.500E+010	0.000
!REF:		
C3H6+HO2<=>C3H6OOH1-2 11000.0	1.000E+011	0.000
C3H6OOH1-3=>OH+CH2O+C2H4 27400.0	3.035E+015	-0.790
!REF:BOZZELLI AND PITZ, 1995		
C3H6OOH2-1<=>C2H3OOH+CH3 38320.0	6.540E+027	-5.140
C3H6OOH1-2=>C2H4+CH2O+OH 48120.0	1.310E+033	-7.010

!REF:ESTIMATE		
C3H6OOH2-2<=>CH3COCH3+OH 1500.0	9.000E+014	0.000
C3H6OOH1-2+O2<=>C3H6OOH1-2O2 0.0	5.000E+012	0.000
C3H6OOH1-3+O2<=>C3H6OOH1-3O2 0.0	4.520E+012	0.000
C3H6OOH2-1+O2<=>C3H6OOH2-1O2 0.0	4.520E+012	0.000
!REF:		
C3H6OOH1-2O2<=>C3KET12+OH 26400.0	6.000E+011	0.000
C3H6OOH1-3O2<=>C3KET13+OH 21400.0	7.500E+010	0.000
C3H6OOH2-1O2<=>C3KET21+OH 23850.0	3.000E+011	0.000
C3H6OOH2-1O2<=>C3H51-2,3OOH 24400.0	1.125E+011	0.000
C3H6OOH1-2O2<=>C3H51-2,3OOH 29400.0	9.000E+011	0.000
!REF: BOZZELLI AND PITZ, 1993.		
C3H51-2,3OOH<=>AC3H5OOH+HO2 17770.0	2.560E+013	-0.490
!REF:		
C3H6OOH1-3O2<=>C3H52-1,3OOH 26850.0	6.000E+011	0.000
!REF:BOZZELLI AND PITZ, 1993.		
C3H52-1,3OOH<=>AC3H5OOH+HO2 17250.0	1.150E+014	-0.630
!REF:		
!C3KET12=>CH3CHO+HCO+OH 43000.0	9.450E+015	0.000
C3KET13=>CH2O+CH2CHO+OH 43000.0	1.000E+016	0.000
!C3KET21=>CH2O+CH3CO+OH 43000.0	1.000E+016	0.000
!REF:ESTIMATE		
!REF:		
!REF:ACETALDEHYDE ANALOG		
C3H5O+O2<=>C2H3CHO+HO2 6000.0	1.000E+012	0.000
!REF:PITZ ESTIMATE		
C2H3OOH<=>CH2CHO+OH 43000.0	8.400E+014	0.000
!REF:!FLOWERS, M. C., J. CHEM. SOC. FAR. TRANS. I 73, 1927 (1977)		
C3H6O1-2<=>C2H4+CH2O 60000.0	6.000E+014	0.000

!REF:WESTBROOK ESTIMATE

C3H6O1-2+OH=>CH2O+C2H3+H2O 0.0	5.000E+012	0.000
C3H6O1-2+H=>CH2O+C2H3+H2 5000.0	2.630E+007	2.000
C3H6O1-2+O=>CH2O+C2H3+OH 5200.0	8.430E+013	0.000
C3H6O1-2+HO2=>CH2O+C2H3+H2O2 15000.0	1.000E+013	0.000
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H 19000.0	1.000E+013	0.000
C3H6O1-2+CH3=>CH2O+C2H3+CH4 10000.0	2.000E+011	0.000

!REF:WESTBROOK AND PITZ ESTIMATE (1983)

C3H6O1-3<=>C2H4+CH2O 60000.0	6.000E+014	0.000
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!REF:PITZ ESTIMATE

C3H6O1-3+OH=>CH2O+C2H3+H2O 0.0	5.000E+012	0.000
C3H6O1-3+O=>CH2O+C2H3+OH 5200.0	8.430E+013	0.000
C3H6O1-3+H=>CH2O+C2H3+H2 5000.0	2.630E+007	2.000
C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H 19000.0	1.000E+013	0.000
C3H6O1-3+HO2=>CH2O+C2H3+H2O2 15000.0	1.000E+013	0.000
C3H6O1-3+CH3=>CH2O+C2H3+CH4 10000.0	2.000E+011	0.000

!REF:

NC3H7O2<=>C3H6+HO2 39510.0	4.308E+036	-7.500
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!REF:NEW TROE FIT FROM TIBOR NAGY

!REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253

C4H10 (+M) <=> C2H5+C2H5 (+M) 92929.0	1.355E+037	-6.036
LOW/ 49578.0/	4.720E+018	0.000
TROE/ 7.998E-002 1.000E-020 3.243E+004 4.858E+003/		

!REF:NEW TROE FIT FROM TIBOR NAGY

!REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253

C4H10 (+M) <=> NC3H7+CH3 (+M) 100330.0	6.600E+052	-10.626
LOW/ 42959.0/	5.340E+017	0.000
TROE/ 9.502E-002 1.000E-020 5.348E+003 4.326E+003/		

!REF:

PC4H9+H<=>C4H10 0.0	3.610E+013	0.000
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SC4H9+H<=>C4H10	3.610E+013	0.000
0.0		
C4H10+O2<=>PC4H9+HO2	6.000E+013	0.000
52340.0		
C4H10+O2<=>SC4H9+HO2	4.000E+013	0.000
49800.0		
!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
C4H10+C3H5-A<=>PC4H9+C3H6	7.940E+011	0.000
20500.0		
C4H10+C3H5-A<=>SC4H9+C3H6	3.160E+011	0.000
16400.0		
C4H10+C2H5<=>PC4H9+C2H6	1.580E+011	0.000
12300.0		
C4H10+C2H5<=>SC4H9+C2H6	1.000E+011	0.000
10400.0		
!REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17,		
174 (1978)		
C4H10+C2H3<=>PC4H9+C2H4	1.000E+012	0.000
18000.0		
C4H10+C2H3<=>SC4H9+C2H4	8.000E+011	0.000
16800.0		
!REF:		
C4H10+CH3<=>PC4H9+CH4	9.040E-001	3.650
7154.0		
C4H10+CH3<=>SC4H9+CH4	3.020E+000	3.460
5481.0		
C4H10+H<=>PC4H9+H2	3.490E+005	2.690
6450.0		
C4H10+H<=>SC4H9+H2	2.600E+006	2.400
4471.0		
C4H10+OH<=>PC4H9+H2O	1.054E+010	0.970
1586.0		
C4H10+OH<=>SC4H9+H2O	9.340E+007	1.610
-35.0		
!REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)		
C4H10+O<=>PC4H9+OH	1.130E+014	0.000
7850.0		
C4H10+O<=>SC4H9+OH	5.620E+013	0.000
5200.0		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-		
7054.		
C4H10+HO2<=>PC4H9+H2O2	4.080E+001	3.590
17160.0		
C4H10+HO2<=>SC4H9+H2O2	1.264E+002	3.370
13720.0		
!REF:DRYER ESTIMATE		
C4H10+CH3O<=>PC4H9+CH3OH	3.000E+011	0.000
7000.0		
C4H10+CH3O<=>SC4H9+CH3OH	6.000E+011	0.000
7000.0		
!REF:ANOLOGY TO CH3O		

C4H10+C2H5O<=>PC4H9+C2H5OH 7000.0	3.000E+011	0.000
C4H10+C2H5O<=>SC4H9+C2H5OH 7000.0	6.000E+011	0.000
!REF:!WESTBROOK AND PITZ ESTIMATE (1983)		
C4H10+PC4H9<=>SC4H9+C4H10 10400.0	1.000E+011	0.000
!REF:ANALOGY TO C2H6+HO2		
C4H10+CH3CO3<=>PC4H9+CH3CO3H 20460.0	1.700E+013	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988		
C4H10+CH3CO3<=>SC4H9+CH3CO3H 17700.0	1.120E+013	0.000
!REF:ANALOGY WITH RH+RO2 --> R+RO2H		
C4H10+O2CHO<=>PC4H9+HO2CHO 20440.0	1.680E+013	0.000
C4H10+O2CHO<=>SC4H9+HO2CHO 17690.0	1.120E+013	0.000
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
!REF:SCALED AS PER CARSTENSEN ET AL		
CH3O2+C4H10<=>CH3O2H+PC4H9 18280.0	1.386E+000	3.970
CH3O2+C4H10<=>CH3O2H+SC4H9 14810.0	2.037E+001	3.580
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C2H5O2+C4H10<=>C2H5O2H+PC4H9 17160.0	4.080E+001	3.590
C2H5O2+C4H10<=>C2H5O2H+SC4H9 13720.0	1.264E+002	3.370
!REF:ANALOGY TO C2H6+HO2		
NC3H7O2+C4H10<=>NC3H7O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988		
NC3H7O2+C4H10<=>NC3H7O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2		
IC3H7O2+C4H10<=>IC3H7O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988		
IC3H7O2+C4H10<=>IC3H7O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2		

PC4H9O2+C3H8<=>PC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
PC4H9O2+C3H8<=>PC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
!REF:ANALOGY TO C2H6+HO2		
PC4H9O2+C4H10<=>PC4H9O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988		
PC4H9O2+C4H10<=>PC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2		
SC4H9O2+C3H8<=>SC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
SC4H9O2+C3H8<=>SC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
SC4H9O2+C4H10<=>SC4H9O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988		
SC4H9O2+C4H10<=>SC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:D.M. MATHEU, W.H. GREEN JR., J.M. GREYDA, INT. J. CHEM. KINET. 35 (2003) 95-119.		
PC4H9<=>SC4H9 37300.0	3.560E+010	0.880
DUP		
PC4H9<=>SC4H9 36600.0	3.800E+010	0.670
DUP		
!REF:		
C2H5+C2H4<=>PC4H9 6130.0	1.320E+004	2.480
C3H6+CH3<=>SC4H9 6130.0	1.760E+004	2.480
C4H8-1+H<=>PC4H9 2620.0	2.500E+011	0.510
C4H8-2+H<=>SC4H9 2620.0	2.500E+011	0.510
C4H8-1+H<=>SC4H9 1230.0	4.240E+011	0.510
!REF:BASED ON KLIPPENSTEIN ET AL. N, IC3H7+O2		
PC4H9+O2<=>C4H8-1+HO2 11960.0	8.370E-001	3.590

SC4H9+O2<=>C4H8-1+HO2 9322.0	5.350E-001	3.710
SC4H9+O2<=>C4H8-2+HO2 9322.0	1.070E+000	3.710
!REF:WESTBROOK AND PITZ ESTIMATE (1983).		
C2H3+C2H5<=>C4H8-1 0.0	9.000E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H5-A+CH3 (+M) <=>C4H8-1 (+M) -262.3	1.000E+014	-0.320
LOW/ 6250.0/	3.910E+060	-12.810
TROE/ 1.040E-001 1.606E+003 6.000E+004 6.118E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/		
!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
H+C4H71-3<=>C4H8-1 0.0	5.000E+013	0.000
!REF:ESTIMATE		
C4H8-1+O2<=>C4H71-3+HO2 37190.0	2.000E+013	0.000
!REF:		
C4H8-1+O<=>C4H71-3+OH 5884.0	1.750E+011	0.700
C4H8-2+O<=>C4H71-3+OH 7550.0	2.190E+011	0.810
!REF:TSANG '91		
C4H8-1+H<=>C4H71-3+H2 2492.0	1.730E+005	2.500
!REF:ESTIMATE		
C4H8-1+H<=>C4H71-4+H2 6756.0	6.651E+005	2.540
C4H8-1+OH<=>C4H71-1+H2O 1637.9	9.010E-001	3.941
C4H8-1+OH<=>C4H71-2+H2O 478.1	1.430E+001	3.534
C4H8-1+OH<=>C4H71-3+H2O -2802.5	6.690E+001	3.475
C4H8-1+OH<=>C4H71-4+H2O -767.0	4.280E+001	3.374
!REF:BASED ON 0.5 * C2H4+OH<=>C2H3+H2O		
!REF:ESTIMATE		
!REF:TSANG '91		
!REF:TSANG '91		
C4H8-1+CH3<=>C4H71-3+CH4 5675.0	2.210E+000	3.500
C4H8-1+CH3<=>C4H71-4+CH4 7154.0	4.520E-001	3.650
!REF:TSANG '91		

C4H8-1+HO2<=>C4H71-3+H2O2 2.700E+004 0.700
5884.0
C4H8-1+HO2<=>C4H71-4+H2O2 2.380E+003 2.550
16490.0

!REF:TSANG '91

C4H8-1+CH3O2<=>C4H71-3+CH3O2H 2.700E+004 0.700
5884.0
C4H8-1+CH3O2<=>C4H71-4+CH3O2H 2.380E+003 2.550
16490.0
C4H8-1+CH3O<=>C4H71-3+CH3OH 4.000E+001 2.900
8609.0
C4H8-1+CH3O<=>C4H71-4+CH3OH 2.170E+011 0.000
6458.0

!REF:DECHAUX, J.C., OXID. COMM. 2, 95 (1981)

C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H 1.000E+011 0.000
8000.0
C4H8-1+C3H5-A<=>C4H71-3+C3H6 7.900E+010 0.000
12400.0

!REF:ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).

C4H71-3+C4H71-3<=>C4H8-1+C4H6 1.600E+012 0.000
0.0
C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H 1.400E+012 0.000
14900.0
C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H 1.400E+012 0.000
14900.0
C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H 1.400E+012 0.000
14900.0
C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H 1.400E+012 0.000
14900.0
C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H 1.400E+012 0.000
14900.0
C4H8-1+CH3O2<=>C4H8O1-2+CH3O 1.000E+012 0.000
14340.0

!REF:ALLARA AND SHAW, 1980, PARALLEL

H+C4H71-3<=>C4H8-2 5.000E+013 0.000
0.0
C4H8-2+O2<=>C4H71-3+HO2 4.000E+013 0.000
39390.0

!REF:TSANG '91

!REF:PLUS DIFFERENCE BETWEEN 10 AND 20 IN ALKANE

C4H8-2+H<=>C4H71-3+H2 4.440E+004 2.810
4414.0
C4H8-2+OH<=>C4H71-3+H2O 5.100E+008 1.400
1250.0
C4H8-2+CH3<=>C4H71-3+CH4 7.140E+000 3.570
7642.0
C4H8-2+HO2<=>C4H71-3+H2O2 5.940E+004 2.570
16140.0
C4H8-2+CH3O2<=>C4H71-3+CH3O2H 5.940E+004 2.570
16140.0

!REF:ESTIMATE

C4H8-2+CH3O<=>C4H71-3+CH3OH 11990.0	1.800E+001	2.950
!REF:!TWICE RATE OF C3H6+HO2		
C4H8-2+C2H5O2<=>C4H71-3+C2H5O2H 14900.0	3.200E+012	0.000
C4H8-2+NC3H7O2<=>C4H71-3+NC3H7O2H 14900.0	3.200E+012	0.000
C4H8-2+IC3H7O2<=>C4H71-3+IC3H7O2H 14900.0	3.200E+012	0.000
C4H8-2+PC4H9O2<=>C4H71-3+PC4H9O2H 14900.0	3.200E+012	0.000
C4H8-2+SC4H9O2<=>C4H71-3+SC4H9O2H 14900.0	3.200E+012	0.000
!REF:ANALOGY TO C3H6+HO2		
C4H8-1+HO2<=>C4H8O1-2+OH 14340.0	1.000E+012	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION		
!REF:SEATTLE, AUGUST, 1988		
C4H8-2+HO2<=>C4H8O2-3+OH 12310.0	5.620E+011	0.000
C4H8-2+CH3O2<=>C4H8O2-3+CH3O 12310.0	5.620E+011	0.000
!REF:TULLY, PRIVATE COMMUNICATION, 1986.		
C4H8-1+OH<=>PC4H8OH -782.0	4.750E+012	0.000
C4H8-2+OH<=>SC4H8OH -782.0	4.750E+012	0.000
PC4H8OH+O2<=>C4H8OH-1O2 0.0	2.000E+012	0.000
SC4H8OH+O2<=>C4H8OH-2O2 0.0	2.000E+012	0.000
!REF:ANALOGY TO PROPENE		
C4H8OH-1O2=>C2H5CHO+CH2O+OH 25000.0	1.000E+016	0.000
C4H8OH-2O2=>OH+CH3CHO+CH3CHO 25000.0	1.000E+016	0.000
C2H2+C2H5<=>C4H71-1 7800.0	2.000E+011	0.000
C3H4-A+CH3<=>C4H71-2 7800.0	2.000E+011	0.000
C2H4+C2H3<=>C4H71-4 7800.0	2.000E+011	0.000
C3H4-P+CH3<=>C4H72-2 7800.0	1.000E+011	0.000
!REF:!ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
C4H6+H<=>C4H71-3 1300.0	4.000E+013	0.000
!REF:ESTIMATE		
C4H71-3+C2H5<=>C4H8-1+C2H4 -131.0	2.590E+012	0.000

C4H71-3+CH3O<=>C4H8-1+CH2O 0.0	2.410E+013	0.000
C4H71-3+O<=>C2H3CHO+CH3 0.0	6.030E+013	0.000
C4H71-3+HO2<=>C4H7O+OH 0.0	9.640E+012	0.000
C4H71-3+CH3O2<=>C4H7O+CH3O 0.0	9.640E+012	0.000
!REF:EDELSON AND ALLARA, 1980		
C3H5-A+C4H71-3<=>C3H6+C4H6 0.0	6.310E+012	0.000
!REF:BALDWIN, BENNETT, AND WALKER, JCS FARADAY I, 76, 2396 (1980)		
C4H71-3+O2<=>C4H6+HO2 0.0	1.000E+009	0.000
!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
H+C4H71-3<=>C4H6+H2 0.0	3.160E+013	0.000
!REF:EDELSON AND ALLARA, 1980		
C2H5+C4H71-3<=>C4H6+C2H6 0.0	3.980E+012	0.000
C2H3+C4H71-3<=>C2H4+C4H6 0.0	3.980E+012	0.000
!REF:ANALOGY TO CH3O2+CH3		
C4H71-3+C2H5O2<=>C4H7O+C2H5O -1200.0	3.800E+012	0.000
IC3H7O2+C4H71-3<=>IC3H7O+C4H7O -1200.0	3.800E+012	0.000
NC3H7O2+C4H71-3<=>NC3H7O+C4H7O -1200.0	3.800E+012	0.000
!REF:ANALOGY TO BATT'S RATE FOR S-BUTOXY DECOMPOSITION		
C4H7O<=>CH3CHO+C2H3 19000.0	7.940E+014	0.000
C4H7O<=>C2H3CHO+CH3 19000.0	7.940E+014	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C4H6<=>C4H5-I+H 112353.0	5.700E+036	-6.270
C4H6<=>C4H5-N+H 123608.0	5.300E+044	-8.620
C4H6<=>C4H4+H2 94700.0	2.500E+015	0.000
C4H6+H<=>C4H5-N+H2 12240.0	1.330E+006	2.530
C4H6+H<=>C4H5-I+H2 9240.0	6.650E+005	2.530
C4H6+H<=>C2H4+C2H3 21647.0	1.460E+030	-4.340
PLOG/ 1.0000	1.460E+030	-4.340
PLOG/ 10.0000	5.450E+030	-4.510
C4H6+H<=>C3H4-P+CH3 7000.0	2.000E+012	0.000

C4H6+H<=>C3H4-A+CH3	2.000E+012	0.000
7000.0		
C4H6+O<=>C4H5-N+OH	7.500E+006	1.900
3740.0		
C4H6+O<=>C4H5-I+OH	7.500E+006	1.900
3740.0		

!REF:WKM

!REF:ADDED TO REDUCE EARLY CO2 PRODUCTION IN C4H6 FLOW REACTOR DUE TO UPDATE

!REF:IN HCCO+O2. BASED ON THE ANALYSIS FOUND IN LASKIN ET AL.		
C4H6+O<=>C2H2+C2H4O1-2	1.000E+008	1.450
-860.0		

!REF:REDUCED THE CH3CHCHCO CHANNEL TO KEEP THE TOTAL K THE SAME.			
C4H6+O<=>CH3CHCHCO+H	5.000E+007	1.450	
-860.0			
C4H6+O<=>CH2CHCHCHO+H	4.500E+008	1.450	
-860.0			
C4H6+OH<=>C4H5-N+H2O	6.200E+006	2.000	
3430.0			
C4H6+OH<=>C4H5-I+H2O	3.100E+006	2.000	
430.0			
C4H6+HO2<=>C4H6O25+OH	1.200E+012	0.000	
14000.0			
C4H6+HO2<=>C2H3CHOCH2+OH	4.800E+012	0.000	
14000.0			
C4H6+CH3<=>C4H5-N+CH4	2.000E+014	0.000	
22800.0			
C4H6+CH3<=>C4H5-I+CH4	1.000E+014	0.000	
19800.0			
C4H6+C2H3<=>C4H5-N+C2H4	5.000E+013	0.000	
22800.0			
C4H6+C2H3<=>C4H5-I+C2H4	2.500E+013	0.000	
19800.0			
C4H6+C3H3<=>C4H5-N+C3H4-A	1.000E+013	0.000	
22500.0			
C4H6+C3H3<=>C4H5-I+C3H4-A	5.000E+012	0.000	
19500.0			
C4H6+C3H5-A<=>C4H5-N+C3H6	1.000E+013	0.000	
22500.0			
C4H6+C3H5-A<=>C4H5-I+C3H6	5.000E+012	0.000	
19500.0			
C4H71-4<=>C4H6+H	2.480E+053	-12.300	
52000.0			
PLOG/ 1.0000	2.480E+053	-12.300	52000.0/
PLOG/ 10.0000	1.850E+048	-10.500	51770.0/
C2H3+C2H2<=>C4H4+H	7.200E+013	-0.480	
6100.0			
PLOG/ 0.0132	7.200E+013	-0.480	6100.0/
PLOG/ 0.0263	5.000E+014	-0.710	6700.0/
PLOG/ 0.1200	4.600E+016	-1.250	8400.0/
PLOG/ 1.0000	2.000E+018	-1.680	10600.0/
PLOG/ 10.0000	4.900E+016	-1.130	11800.0/
C2H3+C2H2<=>C4H5-N	1.100E+031	-7.140	
5600.0			

PLOG/	0.0132	1.100E+031	-7.140	5600.0/	
PLOG/	0.0263	1.100E+032	-7.330	6200.0/	
PLOG/	0.1200	2.400E+031	-6.950	5600.0/	
PLOG/	1.0000	9.300E+038	-8.760	12000.0/	
PLOG/	10.0000	8.100E+037	-8.090	13400.0/	
C2H3+C2H2<=>C4H5-I				5.000E+034	-8.420
7900.0					
PLOG/	0.0132	5.000E+034	-8.420	7900.0/	
PLOG/	0.0263	2.100E+036	-8.780	9100.0/	
PLOG/	0.1200	1.000E+037	-8.770	9800.0/	
PLOG/	1.0000	1.600E+046	-10.980	18600.0/	
PLOG/	10.0000	5.100E+053	-12.640	28800.0/	
C2H3+C2H3<=>C4H6				7.000E+057	-13.820
17629.0					
PLOG/	0.0263	7.000E+057	-13.820	17629.0/	
PLOG/	0.1200	1.500E+052	-11.970	16056.0/	
PLOG/	1.0000	1.500E+042	-8.840	12483.0/	
C2H3+C2H3<=>C4H5-I+H				1.500E+030	-4.950
12958.0					
PLOG/	0.0263	1.500E+030	-4.950	12958.0/	
PLOG/	0.1200	7.200E+028	-4.490	14273.0/	
PLOG/	1.0000	1.200E+022	-2.440	13654.0/	
C2H3+C2H3<=>C4H5-N+H				1.100E+024	-3.280
12395.0					
PLOG/	0.0263	1.100E+024	-3.280	12395.0/	
PLOG/	0.1200	4.600E+024	-3.380	14650.0/	
PLOG/	1.0000	2.400E+020	-2.040	15361.0/	
C4H5-N<=>C4H5-I				2.400E+060	-16.080
47500.0					
PLOG/	0.0132	2.400E+060	-16.080	47500.0/	
PLOG/	0.0263	1.300E+062	-16.380	49600.0/	
PLOG/	0.1200	4.900E+066	-17.260	55400.0/	
PLOG/	1.0000	1.500E+067	-16.890	59100.0/	
PLOG/	10.0000	2.000E+060	-14.460	58600.0/	
C4H5-N+H<=>C4H5-I+H				3.100E+026	-3.350
17423.0					
C4H5-N+H<=>C4H4+H2				1.500E+013	0.000
0.0					
C4H5-N+OH<=>C4H4+H2O				2.000E+012	0.000
0.0					
C4H5-N+HCO<=>C4H6+CO				5.000E+012	0.000
0.0					
C4H5-N+HO2=>C2H3+CH2CO+OH				6.600E+012	0.000
0.0					
C4H5-N+H2O2<=>C4H6+HO2				1.210E+010	0.000
-596.0					
C4H5-N+HO2<=>C4H6+O2				6.000E+011	0.000
0.0					
C4H5-N+O2<=>CH2CHCHCHO+O				3.000E+011	0.290
11.0					
C4H5-N+O2<=>HCO+C2H3CHO				9.200E+016	-1.390
1010.0					
C4H5-I+H<=>C4H4+H2				3.000E+013	0.000
0.0					
C4H5-I+H<=>C3H3+CH3				2.000E+013	0.000
2000.0					
C4H5-I+OH<=>C4H4+H2O				4.000E+012	0.000
0.0					

C4H5-I+HCO<=>C4H6+CO 0.0	5.000E+012	0.000
C4H5-I+HO2<=>C4H6+O2 0.0	6.000E+011	0.000
C4H5-I+HO2=>C2H3+CH2CO+OH 0.0	6.600E+012	0.000
C4H5-I+H2O2<=>C4H6+HO2 -596.0	1.210E+010	0.000
C4H5-I+O2<=>CH2CO+CH2CHO 2500.0	2.160E+010	0.000
C4H5-2<=>C4H5-I 59100.0	1.500E+067	-16.890
C4H5-2+H<=>C4H5-I+H 17423.0	3.100E+026	-3.350
C4H5-2+HO2=>OH+C2H2+CH3CO 0.0	8.000E+011	0.000
C4H5-2+O2<=>CH3CO+CH2CO 2500.0	2.160E+010	0.000
C4H612<=>C4H5-I+H 92600.0	4.200E+015	0.000
C4H612+H<=>C4H6+H 4000.0	2.000E+013	0.000
C4H612+H<=>C4H5-I+H2 2490.0	1.700E+005	2.500
C4H612+H<=>C3H4-A+CH3 2000.0	2.000E+013	0.000
C4H612+H<=>C3H4-P+CH3 2000.0	2.000E+013	0.000
C4H612+CH3<=>C4H5-I+CH4 18500.0	7.000E+013	0.000
C4H612+O<=>CH2CO+C2H4 327.0	1.200E+008	1.650
C4H612+O<=>C4H5-I+OH 5880.0	1.800E+011	0.700
C4H612+OH<=>C4H5-I+H2O -298.0	3.100E+006	2.000
C4H612<=>C4H6 65000.0	3.000E+013	0.000
C4H6-2<=>C4H6 65000.0	3.000E+013	0.000
C4H6-2<=>C4H612 67000.0	3.000E+013	0.000
C4H6-2+H<=>C4H612+H 4000.0	2.000E+013	0.000
C4H6-2+H<=>C4H5-2+H2 2490.0	3.400E+005	2.500
C4H6-2+H<=>CH3+C3H4-P 1000.0	2.600E+005	2.500
C4H6-2<=>H+C4H5-2 87300.0	5.000E+015	0.000
C4H6-2+CH3<=>C4H5-2+CH4 18500.0	1.400E+014	0.000
C2H3CHOCH2<=>C4H6O23 50600.0	2.000E+014	0.000
C4H6O23<=>CH3CHCHCHO 49400.0	1.950E+013	0.000
C4H6O23<=>C2H4+CH2CO 69300.0	5.750E+015	0.000

C4H6O23<=>C2H2+C2H4O1-2				1.000E+016	0.000
75800.0					
C4H6O25<=>C4H4O+H2				5.300E+012	0.000
48500.0					
C4H4O<=>CO+C3H4-P				1.780E+015	0.000
77500.0					
C4H4O<=>C2H2+CH2CO				5.010E+014	0.000
77500.0					
CH3CHCHCHO<=>C3H6+CO				3.900E+014	0.000
69000.0					
CH3CHCHCHO+H<=>CH2CHCHCHO+H2				1.700E+005	2.500
2490.0					
CH3CHCHCHO+H<=>CH3CHCHCO+H2				1.000E+005	2.500
2490.0					
CH3CHCHCHO+H<=>CH3+C2H3CHO				4.000E+021	-2.390
11180.0					
CH3CHCHCHO+H<=>C3H6+HCO				4.000E+021	-2.390
11180.0					
CH3CHCHCHO+CH3<=>CH2CHCHCHO+CH4				2.100E+000	3.500
5675.0					
CH3CHCHCHO+CH3<=>CH3CHCHCO+CH4				1.100E+000	3.500
5675.0					
CH3CHCHCHO+C2H3<=>CH2CHCHCHO+C2H4				2.210E+000	3.500
4682.0					
CH3CHCHCHO+C2H3<=>CH3CHCHCO+C2H4				1.110E+000	3.500
4682.0					
CH3CHCHCO<=>C3H5-S+CO				1.000E+014	0.000
30000.0					
CH3CHCHCO+H<=>CH3CHCHCHO				1.000E+014	0.000
0.0					
CH2CHCHCHO<=>C3H5-A+CO				1.000E+014	0.000
25000.0					
CH2CHCHCHO+H<=>CH3CHCHCHO				1.000E+014	0.000
0.0					
C4H4+H<=>C4H5-N				1.200E+051	-12.570
12300.0					
PLOG/	0.0132	1.200E+051	-12.570	12300.0/	
PLOG/	0.0263	4.200E+050	-12.340	12500.0/	
PLOG/	0.1200	1.100E+050	-11.940	13400.0/	
PLOG/	1.0000	1.300E+051	-11.920	16500.0/	
PLOG/	10.0000	6.200E+045	-10.080	15800.0/	
C4H4+H<=>C4H5-I				6.100E+053	-13.190
14200.0					
PLOG/	0.0132	6.100E+053	-13.190	14200.0/	
PLOG/	0.0263	9.600E+052	-12.850	14300.0/	
PLOG/	0.1200	2.100E+052	-12.440	15500.0/	
PLOG/	1.0000	4.900E+051	-11.920	17700.0/	
PLOG/	10.0000	1.500E+048	-10.580	18800.0/	
C4H4+H<=>C4H3-N+H2				6.650E+005	2.530
12240.0					
C4H4+H<=>C4H3-I+H2				3.330E+005	2.530
9240.0					
C4H4+OH<=>C4H3-N+H2O				3.100E+007	2.000
3430.0					
C4H4+OH<=>C4H3-I+H2O				1.550E+007	2.000
430.0					
C4H4+O<=>C3H3+HCO				6.000E+008	1.450
-860.0					

C3H3+HCCO<=>C4H4+CO 0.0	2.500E+013	0.000
C3H3+CH<=>C4H3-I+H 0.0	5.000E+013	0.000
C3H3+CH2<=>C4H4+H 0.0	5.000E+013	0.000
C3H3+CH3 (+M) <=>C4H612 (+M) 0.0	1.500E+012	0.000
LOW/ 9770.0/	2.600E+057	-11.940
TROE/ 1.750E-001 1.341E+003 6.000E+004 9.770E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/		
C2H2+C2H (+M) <=>C4H3-N (+M) -363.0	8.300E+010	0.899
LOW/ 1871.0/	1.240E+031	-4.718
TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/ 2.50/ C2H4/ 2.50/		
C4H3-N<=>C4H3-I 53000.0	4.100E+043	-9.490
C4H3-N+H<=>C4H3-I+H 10800.0	2.500E+020	-1.670
C4H3-N+H<=>C2H2+H2CC 10014.0	6.300E+025	-3.340
C4H3-N+H<=>C4H4 13070.0	2.000E+047	-10.260
C4H3-N+H<=>C4H2+H2 0.0	3.000E+013	0.000
C4H3-N+OH<=>C4H2+H2O 0.0	2.000E+012	0.000
C2H2+C2H (+M) <=>C4H3-I (+M) -363.0	8.300E+010	0.899
LOW/ 1871.0/	1.240E+031	-4.718
TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/ 2.50/ C2H4/ 2.50/		
C4H3-I+H<=>C2H2+H2CC 10780.0	2.800E+023	-2.550
C4H3-I+H<=>C4H4 12120.0	3.400E+043	-9.010
C4H3-I+H<=>C4H2+H2 0.0	6.000E+013	0.000
C4H3-I+OH<=>C4H2+H2O 0.0	4.000E+012	0.000
C4H3-I+O2<=>HCCO+CH2CO 0.0	7.860E+016	-1.800
!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)		
C4H3-I+CH2<=>C3H4-A+C2H 0.0	2.000E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C2H2+C2H<=>C4H2+H 0.0	9.600E+013	0.000

C4H2+H<=>C4H3-N	1.100E+042	-8.720
15300.0		
C4H2+H<=>C4H3-I	1.100E+030	-4.920
10800.0		
C4H2+OH<=>H2C4O+H	6.600E+012	0.000
-410.0		
H2C4O+H<=>C2H2+HCCO	5.000E+013	0.000
3000.0		
H2C4O+OH<=>CH2CO+HCCO	1.000E+007	2.000
2000.0		
H2CC+C2H2 (+M) <=>C4H4 (+M)	3.500E+005	2.055
-2400.0		
LOW/	1.400E+060	-12.599
7417.0/		
TROE/ 9.800E-001 5.600E+001 5.800E+002 4.164E+003/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/		
3.00/ C2H4/ 3.00/		
H2CC+C2H4<=>C4H6	1.000E+012	0.000
0.0		
!REF:WESTBROOK ESTIMATE		
C4H8O1-2+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0		
C4H8O1-2+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0		
C4H8O1-2+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0		
C4H8O1-2+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0		
C4H8O1-2+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0		
C4H8O1-2+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0		
C4H8O1-3+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0		
C4H8O1-3+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0		
C4H8O1-3+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0		
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0		
C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0		
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0		
C4H8O1-4+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0		
C4H8O1-4+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0		
C4H8O1-4+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0		
C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0		
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0		
C4H8O1-4+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0		

C4H8O2-3+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O2-3+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O2-3+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O2-3+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
!REF:ESTIMATE		
PC4H9+O2<=>PC4H9O2 0.0	4.520E+012	0.000
SC4H9+O2<=>SC4H9O2 0.0	7.540E+012	0.000
!REF:ANALOGY TO CH2O+HO2		
SC4H9O2+CH2O<=>SC4H9O2H+HCO 13600.0	5.600E+012	0.000
SC4H9O2+CH3CHO<=>SC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
!REF:ESTIMATE		
SC4H9O2+HO2<=>SC4H9O2H+O2 -3275.0	1.750E+010	0.000
IC3H7O2+PC4H9<=>IC3H7O+PC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+SC4H9<=>IC3H7O+SC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+PC4H9<=>NC3H7O+PC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+SC4H9<=>NC3H7O+SC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+SC4H9O2=>O2+SC4H9O+SC4H9O 1860.0	1.400E+016	-1.610
SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+CH3O2=>SC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
H2+PC4H9O2<=>H+PC4H9O2H 26030.0	3.010E+013	0.000
H2+SC4H9O2<=>H+SC4H9O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
C2H6+PC4H9O2<=>C2H5+PC4H9O2H 20460.0	1.700E+013	0.000

C2H6+SC4H9O2<=>C2H5+SC4H9O2H 20460.0	1.700E+013	0.000
PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO 9500.0	2.000E+011	0.000
SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO 9500.0	2.000E+011	0.000
!REF:ESTIMATE		
SC4H9O2+CH3<=>SC4H9O+CH3O -1000.0	7.000E+012	0.000
SC4H9O2+C2H5<=>SC4H9O+C2H5O -1000.0	7.000E+012	0.000
SC4H9O2+IC3H7<=>SC4H9O+IC3H7O -1000.0	7.000E+012	0.000
SC4H9O2+NC3H7<=>SC4H9O+NC3H7O -1000.0	7.000E+012	0.000
SC4H9O2+PC4H9<=>SC4H9O+PC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+SC4H9<=>SC4H9O+SC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+C3H5-A<=>SC4H9O+C3H5O -1000.0	7.000E+012	0.000
!REF:ANALOGY TO CH2O+HO2		
PC4H9O2+CH2O<=>PC4H9O2H+HCO 13600.0	5.600E+012	0.000
!REF:HALF OF CH2O+HO2		
PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
PC4H9O2+HO2<=>PC4H9O2H+O2 -3275.0	1.750E+010	0.000
!REF:ANALOGY TO C3H6+HO2		
C3H6+PC4H9O2<=>C3H5-A+PC4H9O2H 13288.1	5.350E-002	4.207
C3H6+SC4H9O2<=>C3H5-A+SC4H9O2H 13288.1	5.350E-002	4.207
!REF:ANALOGY TO C2H4+HO2		
C2H4+PC4H9O2<=>C2H3+PC4H9O2H 30430.0	1.130E+013	0.000
C2H4+SC4H9O2<=>C2H3+SC4H9O2H 30430.0	1.130E+013	0.000
!REF:ANALOGY TO CH3OH+HO2		
CH3OH+PC4H9O2<=>CH2OH+PC4H9O2H 19360.0	6.300E+012	0.000
CH3OH+SC4H9O2<=>CH2OH+SC4H9O2H 19360.0	6.300E+012	0.000
!REF:HALF OF CH2O+HO2		
C2H3CHO+PC4H9O2<=>C2H3CO+PC4H9O2H 13600.0	2.800E+012	0.000
C2H3CHO+SC4H9O2<=>C2H3CO+SC4H9O2H 13600.0	2.800E+012	0.000

!REF:ANALOGY TO CH4+HO2		
CH4+PC4H9O2<=>CH3+PC4H9O2H 24640.0	1.120E+013	0.000
CH4+SC4H9O2<=>CH3+SC4H9O2H 24640.0	1.120E+013	0.000
!REF:ESTIMATE		
C4H71-3+PC4H9O2<=>C4H7O+PC4H9O -1000.0	7.000E+012	0.000
C4H71-3+SC4H9O2<=>C4H7O+SC4H9O -1000.0	7.000E+012	0.000
!REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H		
H2O2+PC4H9O2<=>HO2+PC4H9O2H 10000.0	2.400E+012	0.000
H2O2+SC4H9O2<=>HO2+SC4H9O2H 10000.0	2.400E+012	0.000
!REF:		
PC4H9O2+PC4H9O2=>O2+PC4H9O+PC4H9O 1860.0	1.400E+016	-1.610
PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+CH3O2=>PC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
!REF:ESTIMATE		
PC4H9O2+CH3<=>PC4H9O+CH3O -1000.0	7.000E+012	0.000
PC4H9O2+C2H5<=>PC4H9O+C2H5O -1000.0	7.000E+012	0.000
PC4H9O2+IC3H7<=>PC4H9O+IC3H7O -1000.0	7.000E+012	0.000
PC4H9O2+NC3H7<=>PC4H9O+NC3H7O -1000.0	7.000E+012	0.000
PC4H9O2+PC4H9<=>PC4H9O+PC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+SC4H9<=>PC4H9O+SC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+C3H5-A<=>PC4H9O+C3H5O -1000.0	7.000E+012	0.000
PC4H9+HO2<=>PC4H9O+OH -1000.0	7.000E+012	0.000
SC4H9+HO2<=>SC4H9O+OH -1000.0	7.000E+012	0.000
CH3O2+PC4H9<=>CH3O+PC4H9O -1000.0	7.000E+012	0.000
CH3O2+SC4H9<=>CH3O+SC4H9O -1000.0	7.000E+012	0.000

!REF:		
PC4H9O2H<=>PC4H9O+OH	1.500E+016	0.000
42500.0		
!REF:PITZ ESTIMATE		
SC4H9O+OH<=>SC4H9O2H	1.000E+015	-0.800
0.0		
!REF:		
NC3H7+CH2O<=>PC4H9O	5.000E+010	0.000
3457.0		
CH3+C2H5CHO<=>SC4H9O	5.000E+010	0.000
9043.0		
C2H5+CH3CHO<=>SC4H9O	3.330E+010	0.000
6397.0		
!REF:		
PC4H9O2<=>C4H8OOH1-2	2.000E+011	0.000
31850.0		
PC4H9O2<=>C4H8OOH1-3	2.500E+010	0.000
20850.0		
PC4H9O2<=>C4H8OOH1-4	4.688E+009	0.000
22350.0		
SC4H9O2<=>C4H8OOH2-1	3.000E+011	0.000
34500.0		
SC4H9O2<=>C4H8OOH2-3	2.000E+011	0.000
31850.0		
SC4H9O2<=>C4H8OOH2-4	3.750E+010	0.000
24400.0		
PC4H9O2<=>C4H8-1+HO2	4.308E+036	-7.500
39510.0		
SC4H9O2<=>C4H8-1+HO2	5.980E+042	-9.430
41530.0		
SC4H9O2<=>C4H8-2+HO2	4.308E+036	-7.500
39510.0		
!REF:		
C4H8-1+HO2<=>C4H8OOH1-2	1.000E+011	0.000
11000.0		
C4H8-1+HO2<=>C4H8OOH2-1	1.000E+011	0.000
11750.0		
C4H8-2+HO2<=>C4H8OOH2-3	1.000E+011	0.000
11750.0		
!REF:GREEN 2003		
C4H8OOH1-2<=>C4H8O1-2+OH	1.380E+012	0.000
15900.0		
C4H8OOH1-3<=>C4H8O1-3+OH	2.040E+011	0.000
19500.0		
C4H8OOH1-4<=>C4H8O1-4+OH	5.130E+010	0.000
14800.0		
C4H8OOH2-1<=>C4H8O1-2+OH	3.980E+012	0.000
17000.0		
C4H8OOH2-3<=>C4H8O2-3+OH	1.380E+012	0.000
15900.0		
C4H8OOH2-4<=>C4H8O1-3+OH	4.470E+011	0.000
21900.0		

!REF:ESTIMATE

C4H8OOH1-1<=>NC3H7CHO+OH 1500.0	9.000E+014	0.000
C4H8OOH2-2<=>C2H5COCH3+OH 1500.0	9.000E+014	0.000

!REF:GREEN 2003

C4H8OOH1-3=>OH+CH2O+C3H6 29900.0	6.635E+013	-0.160
C4H8OOH2-4=>OH+CH3CHO+C2H4 26790.0	1.945E+018	-1.630

!REF:ESTIMATE?

C4H8OOH1-2+O2<=>C4H8OOH1-2O2 0.0	7.540E+012	0.000
C4H8OOH1-3+O2<=>C4H8OOH1-3O2 0.0	7.540E+012	0.000
C4H8OOH1-4+O2<=>C4H8OOH1-4O2 0.0	4.520E+012	0.000
C4H8OOH2-1+O2<=>C4H8OOH2-1O2 0.0	4.520E+012	0.000
C4H8OOH2-3+O2<=>C4H8OOH2-3O2 0.0	7.540E+012	0.000
C4H8OOH2-4+O2<=>C4H8OOH2-4O2 0.0	4.520E+012	0.000

!REF:

C4H8OOH1-2O2<=>NC4KET12+OH 31500.0	2.000E+011	0.000
C4H8OOH1-3O2<=>NC4KET13+OH 21400.0	2.500E+010	0.000
C4H8OOH1-4O2<=>NC4KET14+OH 19350.0	3.125E+009	0.000
C4H8OOH2-1O2<=>NC4KET21+OH 28850.0	1.000E+011	0.000
C4H8OOH2-3O2<=>NC4KET23+OH 28850.0	1.000E+011	0.000
C4H8OOH2-4O2<=>NC4KET24+OH 17850.0	1.250E+010	0.000

!REF:

NC4KET12=>C2H5CHO+HCO+OH 41600.0	1.050E+016	0.000
NC4KET13=>CH3CHO+CH2CHO+OH 41600.0	1.050E+016	0.000
NC4KET14=>CH2CH2CHO+CH2O+OH 42000.0	1.500E+016	0.000
NC4KET21=>CH2O+C2H5CO+OH 42000.0	1.500E+016	0.000
NC4KET23=>CH3CHO+CH3CO+OH 41600.0	1.050E+016	0.000
NC4KET24=>CH2O+CH3COCH2+OH 42000.0	1.500E+016	0.000

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995

C2H5COCH3+OH<=>CH2CH2COCH3+H2O 1586.0	7.550E+009	0.970
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!REF:ANALOGY TO C2H5COC2H5+OH<=>PRODUCTS; CURRAN 1995
C2H5COCH3+OH<=>CH3CHCOCH3+H2O 8.450E+011 0.000
-228.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995
C2H5COCH3+OH<=>C2H5COCH2+H2O 5.100E+011 0.000
1192.0

!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995
C2H5COCH3+HO2<=>CH2CH2COCH3+H2O2 2.380E+004 2.550
16490.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+HO2<=>CH3CHCOCH3+H2O2 2.000E+011 0.000
8698.0
C2H5COCH3+HO2<=>C2H5COCH2+H2O2 2.380E+004 2.550
14690.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+O<=>CH2CH2COCH3+OH 2.250E+013 0.000
7700.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+O<=>CH3CHCOCH3+OH 3.070E+013 0.000
3400.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995
C2H5COCH3+O<=>C2H5COCH2+OH 5.000E+012 0.000
5962.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+H<=>CH2CH2COCH3+H2 9.160E+006 2.000
7700.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+H<=>CH3CHCOCH3+H2 4.460E+006 2.000
3200.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995
C2H5COCH3+H<=>C2H5COCH2+H2 9.300E+012 0.000
6357.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+O2<=>CH2CH2COCH3+HO2 2.050E+013 0.000
51310.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+O2<=>CH3CHCOCH3+HO2 1.550E+013 0.000
41970.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995

C2H5COCH3+O2<=>C2H5COCH2+HO2 49150.0	2.050E+013	0.000
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+CH3<=>CH2CH2COCH3+CH4 7172.0	3.190E+001	3.170
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3<=>CH3CHCOCH3+CH4 3680.0	1.740E+000	3.460
!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+CH3<=>C2H5COCH2+CH4 9630.0	1.620E+011	0.000
!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		
C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH 6460.0	2.170E+011	0.000
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH 2771.0	1.450E+011	0.000
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH 4660.0	2.170E+011	0.000
!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		
C2H5COCH3+CH3O2<=>CH2CH2COCH3+CH3O2H 19380.0	3.010E+012	0.000
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O2<=>CH3CHCOCH3+CH3O2H 15250.0	2.000E+012	0.000
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O2<=>C2H5COCH2+CH3O2H 17580.0	3.010E+012	0.000
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+C2H3<=>CH2CH2COCH3+C2H4 10400.0	5.000E+011	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+C2H3<=>CH3CHCOCH3+C2H4 3400.0	3.000E+011	0.000
!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+C2H3<=>C2H5COCH2+C2H4 4278.0	6.150E+010	0.000
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		

C2H5COCH3+C2H5<=>CH2CH2COCH3+C2H6 13400.0	5.000E+010	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+C2H5<=>CH3CHCOCH3+C2H6 8600.0	3.000E+010	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+C2H5<=>C2H5COCH2+C2H6 11600.0	5.000E+010	0.000
!REF: CURRAN AND GAFFURI, 1995		
CH3CHCOCH3+O2<=>CH3CHOOOCOCH3 0.0	1.000E+011	0.000
CH3CHOOOCOCH3<=>CH2CHOOHCOCH3 29700.0	8.900E+012	0.000
C2H3COCH3+HO2<=>CH2CHOOHCOCH3 7800.0	7.000E+010	0.000
!REF:		
CH2CH2COCH3<=>C2H4+CH3CO 18000.0	1.000E+014	0.000
!REF: WKM 19/ 04/ 2010		
C2H5COCH2<=>CH2CO+C2H5 35000.0	1.000E+014	0.000
!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS		
!C2H3COCH3+H<=>CH3CHCOCH3 1200.0	5.000E+012	0.000
!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS		
CH3CHCO+CH3<=>CH3CHCOCH3 7800.0	1.230E+011	0.000
!REF:ANALOGY WITH ACETALDEHYDE		
NC3H7CHO+O2<=>NC3H7CO+HO2 37560.0	1.200E+005	2.500
NC3H7CHO+OH<=>NC3H7CO+H2O -1300.0	2.000E+006	1.800
NC3H7CHO+H<=>NC3H7CO+H2 2320.0	4.140E+009	1.120
NC3H7CHO+O<=>NC3H7CO+OH 1868.0	5.940E+012	0.000
!REF:HALF OF CH2O+HO2		
NC3H7CHO+HO2<=>NC3H7CO+H2O2 10200.0	4.090E+004	2.500
!REF:ANALOGY WITH ACETALDEHYDE		
NC3H7CHO+CH3<=>NC3H7CO+CH4 3210.0	2.890E-003	4.620
NC3H7CHO+CH3O<=>NC3H7CO+CH3OH 3300.0	1.000E+012	0.000
!REF:PITZ ESTIMATE		

NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H 4.090E+004 2.500
10200.0

!REF:CURRAN ESTIMATE

NC3H7CHO+OH<=>C3H6CHO-1+H2O 5.280E+009 0.970
1586.0

NC3H7CHO+OH<=>C3H6CHO-2+H2O 4.680E+007 1.610
-35.0

NC3H7CHO+OH<=>C3H6CHO-3+H2O 5.520E+002 3.120
-1176.0

NC3H7CHO+HO2<=>C3H6CHO-1+H2O2 2.379E+004 2.550
16490.0

NC3H7CHO+HO2<=>C3H6CHO-2+H2O2 9.640E+003 2.600
13910.0

NC3H7CHO+HO2<=>C3H6CHO-3+H2O2 3.440E+012 0.050
17880.0

!REF:CURRAN ESTIMATE

NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H 2.379E+004 2.550
16490.0

NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H 9.640E+003 2.600
13910.0

NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H 3.440E+012 0.050
17880.0

NC3H7CO<=>NC3H7+CO 1.000E+011 0.000
9600.0

!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95.

C3H6CHO-1<=>C2H4+CH2CHO 7.400E+011 0.000
21970.0

!REF:CURRAN ESTIMATE

C2H5CHCO+H<=>C3H6CHO-3 5.000E+012 0.000
1200.0

C2H3CHO+CH3<=>C3H6CHO-3 1.230E+011 0.000
7800.0

SC3H5CHO+H<=>C3H6CHO-2 5.000E+012 0.000
2900.0

C3H6+HCO<=>C3H6CHO-2 1.000E+011 0.000
6000.0

C2H5CHCO+OH<=>NC3H7+CO2 3.730E+012 0.000
-1010.0

C2H5CHCO+H<=>NC3H7+CO 4.400E+012 0.000
1459.0

C2H5CHCO+O<=>C3H6+CO2 3.200E+012 0.000
-437.0

!REF:ANALOGY WITH ACETALDEHYDE

SC3H5CHO+OH<=>SC3H5CO+H2O 2.690E+010 0.760
-340.0

!REF:PITZ ESTIMATE

C3H5-S+CO<=>SC3H5CO 5.000E+012 0.000
8000.0

!REF:ANALOGY WITH IC3H5CHO+X --> IC3H5CO+HX

SC3H5CHO+HO2<=>SC3H5CO+H2O2 1.000E+012 0.000
11920.0

SC3H5CHO+CH3<=>SC3H5CO+CH4 8700.0	3.980E+012	0.000
SC3H5CHO+O<=>SC3H5CO+OH 1389.0	7.180E+012	0.000
SC3H5CHO+O2<=>SC3H5CO+HO2 37600.0	4.000E+013	0.000
SC3H5CHO+H<=>SC3H5CO+H2 2600.0	2.600E+012	0.000

!REF:CURRAN ESTIMATE

C2H3COCH3+OH<=>CH3CHO+CH3CO 0.0	1.000E+011	0.000
C2H3COCH3+OH=>CH2CO+C2H3+H2O 1192.0	5.100E+011	0.000
C2H3COCH3+HO2=>CH2CHO+CH3CO+OH 7949.0	6.030E+009	0.000
C2H3COCH3+HO2=>CH2CO+C2H3+H2O2 20460.0	8.500E+012	0.000
C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O 17050.0	3.970E+011	0.000
C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H 17580.0	3.010E+012	0.000

CH2CHOOHCOCH3=>CH2CHO+CH3CO+OH	2.282E+8	1.290	9890
!C2H3COCH3+OH=>CH2CO+C2H3+H2O	1.10E+05	2.4	-1505.736138
C2H3COCH3+H=>CH2CO+C2H3+H2	7.76E+13	0	11591.5
C2H3COCH3+CH3=>CH2CO+C2H3+CH4	4.75E12	0.000	13694.7
C2H3COCH3+OH=>CJC(OH)C(*O)C	1.56E8	1.290	-2652.9
CJC(OH)C(*O)C=>C2H3OH+CH3CO	1.68E14	0.000	22083.6

!REF:NEW FIT FROM TIBOR NAGY BASED ON:

!REF:OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253

IC4H10(+M)<=>CH3+IC3H7(+M) 91495.0	2.520E+031	-4.102
LOW/ 52576.0/	2.410E+019	0.000
TROE/ 3.662E-001 8.153E+002 6.079E+001 1.000E+020/		

!REF:OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253.

IC4H10<=>TC4H9+H 145300.0	2.510E+098	-23.810
IC4H10<=>IC4H9+H 147600.0	9.850E+095	-23.110

!REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)

IC4H10+H<=>TC4H9+H2 2583.0	6.020E+005	2.400
IC4H10+H<=>IC4H9+H2 6756.0	1.810E+006	2.540
IC4H10+CH3<=>TC4H9+CH4 4598.0	9.040E-001	3.460
IC4H10+CH3<=>IC4H9+CH4 7154.0	1.360E+000	3.650

!REF:JOE MICHAELS SYMP. PAPER 2008.

IC4H10+OH<=>TC4H9+H2O -1659.0	2.925E+004	2.531
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IC4H10+OH<=>IC4H9+H2O -168.9	6.654E+004	2.665
!REF:ALLARA AND SHAW ANALOG		
IC4H10+C2H5<=>IC4H9+C2H6 10400.0	1.510E+012	0.000
!REF:FROM ISOBUTYL RATE		
IC4H10+C2H5<=>TC4H9+C2H6 7900.0	1.000E+011	0.000
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
IC4H10+HO2<=>IC4H9+H2O2 17160.0	6.120E+001	3.590
!REF: X0.666		
IC4H10+HO2<=>TC4H9+H2O2 12090.0	4.332E+002	3.010
!REF:FIT TO TSANG 90 AND COHEN DATA		
!REF:NIST STANDARD REFERENCE DATABASE 17 -2Q98		
IC4H10+O<=>TC4H9+OH 1150.0	1.968E+005	2.402
IC4H10+O<=>IC4H9+OH 5136.0	4.046E+007	2.034
!REF:ANALOGY TO C3H8+CH3O		
IC4H10+CH3O<=>IC4H9+CH3OH 7000.0	4.800E+011	0.000
!REF:TAMURA ESTIMATE		
IC4H10+CH3O<=>TC4H9+CH3OH 2800.0	1.900E+010	0.000
!REF:		
IC4H10+O2<=>IC4H9+HO2 52290.0	9.000E+013	0.000
IC4H10+O2<=>TC4H9+HO2 48200.0	1.000E+013	0.000
!REF:BASED ON (SCALED AS PER CARSTENSEN		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
IC4H10+CH3O2<=>IC4H9+CH3O2H 18280.0	2.079E+000	3.970
!REF:SCOTT AND WALKER C&F 129(4) 365--377 2002 (*1.5)		
IC4H10+C2H5O2<=>IC4H9+C2H5O2H 20460.0	2.550E+013	0.000
!REF:ANALOGY TO C2H6+HO2		
IC4H10+CH3CO3<=>IC4H9+CH3CO3H 20460.0	2.550E+013	0.000
IC4H10+NC3H7O2<=>IC4H9+NC3H7O2H 20460.0	2.550E+013	0.000

IC4H10+IC3H7O2<=>IC4H9+IC3H7O2H 20460.0	2.550E+013	0.000
IC4H10+IC4H9O2<=>IC4H9+IC4H9O2H 20460.0	2.550E+013	0.000
IC4H10+TC4H9O2<=>IC4H9+TC4H9O2H 20460.0	2.550E+013	0.000
!REF:ANALOGY WITH RH+RO2 --> R+RO2H		
IC4H10+O2CHO<=>IC4H9+HO2CHO 20440.0	2.520E+013	0.000
IC4H10+O2CHO<=>TC4H9+HO2CHO 16010.0	2.800E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H10+SC4H9O2<=>IC4H9+SC4H9O2H 20460.0	2.250E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+SC4H9O2<=>TC4H9+SC4H9O2H 16000.0	2.800E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H10+PC4H9O2<=>IC4H9+PC4H9O2H 20460.0	2.250E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+PC4H9O2<=>TC4H9+PC4H9O2H 16000.0	2.800E+012	0.000
!REF:BASED ON (SCALED AS PER CARSTENSEN		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047- 7054.		
IC4H10+CH3O2<=>TC4H9+CH3O2H 13190.0	1.366E+002	3.120
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+C2H5O2<=>TC4H9+C2H5O2H 16000.0	2.800E+012	0.000
IC4H10+CH3CO3<=>TC4H9+CH3CO3H 16000.0	2.800E+012	0.000
IC4H10+NC3H7O2<=>TC4H9+NC3H7O2H 16000.0	2.800E+012	0.000
IC4H10+IC3H7O2<=>TC4H9+IC3H7O2H 16000.0	2.800E+012	0.000
IC4H10+IC4H9O2<=>TC4H9+IC4H9O2H 16000.0	2.800E+012	0.000
IC4H10+TC4H9O2<=>TC4H9+TC4H9O2H 16000.0	2.800E+012	0.000
!REF:WESTBROOK AND PITZ ESTIMATE (1983)		
IC4H10+IC4H9<=>TC4H9+IC4H10 7900.0	2.500E+010	0.000
!REF:ESTIMATE		

IC4H9+HO2<=>IC4H9O+OH -1000.0	7.000E+012	0.000
TC4H9+HO2<=>TC4H9O+OH -1000.0	7.000E+012	0.000
CH3O2+IC4H9<=>CH3O+IC4H9O -1000.0	7.000E+012	0.000
CH3O2+TC4H9<=>CH3O+TC4H9O -1000.0	7.000E+012	0.000
!REF:		
IC4H9<=>TC4H9 34600.0	3.560E+010	0.880
!REF:CURRAN INT J CHEM KINET 38:250-275, 2006		
!IC4H8+H<=>IC4H9 2620.0	6.250E+011	0.510
!C3H6+CH3<=>IC4H9 6850.0	1.890E+003	2.670
!H+IC4H8<=>TC4H9 1230.0	1.060E+012	0.510
!REF:		
TC4H9+O2<=>IC4H8+HO2 11960.0	8.370E-001	3.590
IC4H9+O2<=>IC4H8+HO2 9322.0	1.070E+000	3.710
NC3H7O2+IC4H9<=>NC3H7O+IC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+TC4H9<=>NC3H7O+TC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+IC4H7<=>NC3H7O+IC4H7O -1000.0	7.000E+012	0.000
SC4H9O2+IC4H9<=>SC4H9O+IC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+TC4H9<=>SC4H9O+TC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+IC4H9<=>PC4H9O+IC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+TC4H9<=>PC4H9O+TC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+IC4H7<=>PC4H9O+IC4H7O -1000.0	7.000E+012	0.000
SC4H9O2+IC4H7<=>SC4H9O+IC4H7O -1000.0	7.000E+012	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION, SEATTLE, AUGUST, 1988.		
IC4H9O2+C4H10<=>IC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
TC4H9O2+C4H10<=>TC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C4H10<=>IC4H9O2H+PC4H9 20460.0	1.700E+013	0.000
TC4H9O2+C4H10<=>TC4H9O2H+PC4H9 20460.0	1.700E+013	0.000

!REF:ESTIMATE

IC3H7O2+IC4H9<=>IC3H7O+IC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+TC4H9<=>IC3H7O+TC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+IC4H7<=>IC3H7O+IC4H7O -1000.0	7.000E+012	0.000

!REF:ANALOGY TO C3H6+HO2.

IC4H9O2+C3H6<=>IC4H9O2H+C3H5-A 13288.1	5.350E-002	4.207
TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A 13288.1	5.350E-002	4.207

!REF:WESTBROOK ESTIMATE

IC4H9O2+IC4H8<=>IC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
TC4H9O2+IC4H8<=>TC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
PC4H9O2+IC4H8<=>PC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
SC4H9O2+IC4H8<=>SC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
IC3H7O2+IC4H8<=>IC3H7O2H+IC4H7 14900.0	1.400E+012	0.000
NC3H7O2+IC4H8<=>NC3H7O2H+IC4H7 14900.0	1.400E+012	0.000
IC4H9O2+C4H8-1<=>IC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
TC4H9O2+C4H8-1<=>TC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
IC4H9O2+C4H8-2<=>IC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
TC4H9O2+C4H8-2<=>TC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
CC4H8O+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
CC4H8O+H=>CH2O+C3H5-A+H2 5000.0	3.510E+007	2.000
CC4H8O+O=>CH2O+C3H5-A+OH 5200.0	1.124E+014	0.000
CC4H8O+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
CC4H8O+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
CC4H8O+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000

!REF:PITZ ESTIMATE

C2H4+TC4H9O2<=>C2H3+TC4H9O2H 27132.0	8.590E+000	3.754
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!REF:WESTBROOK ESTIMATE

TC4H9O2+CH4<=>TC4H9O2H+CH3 20460.0	1.130E+013	0.000
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!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986

H2+TC4H9O2<=>H+TC4H9O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
TC4H9O2+C2H6<=>TC4H9O2H+C2H5 20460.0	1.700E+013	0.000
TC4H9O2+C3H8<=>TC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
TC4H9O2+C3H8<=>TC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
TC4H9O2+CH3OH<=>TC4H9O2H+CH2OH 19360.0	6.300E+012	0.000
TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH 19360.0	6.300E+012	0.000
TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH 15000.0	4.200E+012	0.000
!REF:HALF OF CH2O+HO2		
IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
IC4H9O2+C2H3CHO<=>IC4H9O2H+C2H3CO 13600.0	2.800E+012	0.000
TC4H9O2+C2H3CHO<=>TC4H9O2H+C2H3CO 13600.0	2.800E+012	0.000
IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO 13600.0	2.800E+012	0.000
TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO 13600.0	2.800E+012	0.000
!REF:ESTIMATE?		
IC4H9O2+HO2<=>IC4H9O2H+O2 -3275.0	1.750E+010	0.000
TC4H9O2+HO2<=>TC4H9O2H+O2 -3275.0	1.750E+010	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+H2O2<=>IC4H9O2H+HO2 10000.0	2.400E+012	0.000
TC4H9O2+H2O2<=>TC4H9O2H+HO2 10000.0	2.400E+012	0.000
IC4H9O2+CH2O<=>IC4H9O2H+HCO 9000.0	1.300E+011	0.000
TC4H9O2+CH2O<=>TC4H9O2H+HCO 9000.0	1.300E+011	0.000
!REF:		
IC4H9O2+CH3O2=>IC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+CH3O2=>TC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610

TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
IC4H9O2+IC4H9O2=>O2+IC4H9O+IC4H9O 1860.0	1.400E+016	-1.610
IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+TC4H9O2=>O2+TC4H9O+TC4H9O 1860.0	1.400E+016	-1.610
IC4H9O2+PC4H9O2=>IC4H9O+PC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+PC4H9O2=>TC4H9O+PC4H9O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+HO2=>IC4H9O+OH+O2 1860.0	1.400E+016	-1.610
TC4H9O2+HO2=>TC4H9O+OH+O2 1860.0	1.400E+016	-1.610

!REF:ESTIMATE

IC4H9O2+CH3<=>IC4H9O+CH3O -1000.0	7.000E+012	0.000
IC4H9O2+C2H5<=>IC4H9O+C2H5O -1000.0	7.000E+012	0.000
IC4H9O2+IC3H7<=>IC4H9O+IC3H7O -1000.0	7.000E+012	0.000
IC4H9O2+NC3H7<=>IC4H9O+NC3H7O -1000.0	7.000E+012	0.000
IC4H9O2+PC4H9<=>IC4H9O+PC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+SC4H9<=>IC4H9O+SC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+IC4H9<=>IC4H9O+IC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+TC4H9<=>IC4H9O+TC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+C3H5-A<=>IC4H9O+C3H5O -1000.0	7.000E+012	0.000
IC4H9O2+C4H71-3<=>IC4H9O+C4H7O -1000.0	7.000E+012	0.000
IC4H9O2+IC4H7<=>IC4H9O+IC4H7O -1000.0	7.000E+012	0.000
TC4H9O2+CH3<=>TC4H9O+CH3O -1000.0	7.000E+012	0.000
TC4H9O2+C2H5<=>TC4H9O+C2H5O -1000.0	7.000E+012	0.000
TC4H9O2+IC3H7<=>TC4H9O+IC3H7O -1000.0	7.000E+012	0.000

TC4H9O2+NC3H7<=>TC4H9O+NC3H7O -1000.0	7.000E+012	0.000
TC4H9O2+PC4H9<=>TC4H9O+PC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+SC4H9<=>TC4H9O+SC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+IC4H9<=>TC4H9O+IC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+TC4H9<=>TC4H9O+TC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+C3H5-A<=>TC4H9O+C3H5O -1000.0	7.000E+012	0.000
TC4H9O2+C4H71-3<=>TC4H9O+C4H7O -1000.0	7.000E+012	0.000
!REF:PITZ ESTIMATE: ANALOGY WITH C2H4+CH3O2		
IC4H9O2+C2H4<=>IC4H9O2H+C2H3 27132.0	8.590E+000	3.754
!REF:WESTBROOK ESTIMATE		
IC4H9O2+CH4<=>IC4H9O2H+CH3 20460.0	1.130E+013	0.000
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
H2+IC4H9O2<=>H+IC4H9O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C2H6<=>IC4H9O2H+C2H5 20460.0	1.700E+013	0.000
IC4H9O2+C3H8<=>IC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
IC4H9O2+C3H8<=>IC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
IC4H9O2+CH3OH<=>IC4H9O2H+CH2OH 19360.0	6.300E+012	0.000
IC4H9O2+C2H5OH<=>IC4H9O2H+PC2H4OH 19360.0	6.300E+012	0.000
IC4H9O2+C2H5OH<=>IC4H9O2H+SC2H4OH 15000.0	4.200E+012	0.000
!REF:		
IC4H9O2H<=>IC4H9O+OH 42500.0	1.500E+016	0.000
TC4H9O2H<=>TC4H9O+OH 42540.0	5.950E+015	0.000
!REF:ANALOGY CH3O+X --> CH2O+HX TSANG/ HAMPSON 86		
IC4H9O+HO2<=>IC3H7CHO+H2O2 0.0	1.000E+012	0.000
IC4H9O+OH<=>IC3H7CHO+H2O 0.0	1.810E+013	0.000
IC4H9O+CH3<=>IC3H7CHO+CH4 0.0	2.400E+013	0.000
IC4H9O+O<=>IC3H7CHO+OH 0.0	6.000E+012	0.000
IC4H9O+H<=>IC3H7CHO+H2 0.0	1.990E+013	0.000

!REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006		
IC3H7CHO+H<=>IC4H9O	1.000E+012	0.000
5860.0		
CH2O+IC3H7<=>IC4H9O	5.000E+010	0.000
2330.0		
CH3COCH3+CH3<=>TC4H9O	1.500E+011	0.000
11900.0		
!REF:!ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503 (1985).		
IC4H9O+O2<=>IC3H7CHO+HO2	1.930E+011	0.000
1660.0		
!REF:PITZ ESTIMATE		
TC4H9O+O2<=>IC4H8O+HO2	8.100E+011	0.000
4700.0		
!REF:FLOWERS, M.C.; PARKER, R.M. INTL. J. CHEM. KINET. 443-452, 1971.		
!REF: X 2.0		
IC4H8O<=>IC3H7CHO	4.180E+013	0.000
52720.0		
!REF:		
IC4H8O+OH<=>IC3H6CHO+H2O	1.250E+012	0.000
0.0		
IC4H8O+H<=>IC3H6CHO+H2	1.250E+012	0.000
0.0		
IC4H8O+HO2<=>IC3H6CHO+H2O2	2.500E+012	0.000
15000.0		
IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H	2.500E+012	0.000
19000.0		
IC4H8O+CH3<=>IC3H6CHO+CH4	5.000E+010	0.000
10000.0		
IC4H8O+O<=>IC3H6CHO+OH	1.250E+012	0.000
0.0		
!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES		
TC3H6CHO+H<=>IC3H7CHO	2.000E+014	0.000
0.0		
!REF:TSANG J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
IC3H7+HCO<=>IC3H7CHO	1.810E+013	0.000
0.0		
!REF:		
IC3H7CHO+HO2<=>IC3H7CO+H2O2	3.000E+012	0.000
11920.0		
!REF:BALDWIN, R.R.; WALKER, R.W.		
!REF:SYMP. INTL. COMB. PROC. 1979, 17, 525.		
IC3H7CHO+HO2<=>TC3H6CHO+H2O2	8.000E+010	0.000
11920.0		
!REF:BIRRELL, R.N.; TROTMAN-DICKENSON, A.F. J. CHEM. SOC. 1960, 2059		
IC3H7CHO+CH3<=>IC3H7CO+CH4	3.980E+012	0.000
8700.0		

!REF:SINGLETON, D.L. ET AL. CAN. J. CHEM. 1977, 55, 3321.
 IC3H7CHO+O<=>IC3H7CO+OH 7.180E+012 0.000
 1389.0

!REF:!BALDWIN, R.R. ET AL. J. CHEM. SOC. FAR. TRANS. 1979, 75, 1433
 IC3H7CHO+O2<=>IC3H7CO+HO2 4.000E+013 0.000
 37600.0

!REF:SEMMES ET AL. INTL. J. CHEM. KINET. 1985, 17, 303.
 IC3H7CHO+OH<=>IC3H7CO+H2O 2.690E+010 0.760
 -340.0
 IC3H7CHO+OH<=>TC3H6CHO+H2O 1.684E+012 0.000
 -781.0

!REF: CURRAN ESTIMATE
 IC3H7CHO+H<=>IC3H7CO+H2 2.600E+012 0.000
 2600.0
 IC3H7CHO+OH<=>IC3H6CHO+H2O 3.120E+006 2.000
 -298.0
 IC3H7CHO+HO2<=>IC3H6CHO+H2O2 2.740E+004 2.550
 15500.0
 IC3H7CHO+CH3O2<=>IC3H6CHO+CH3O2H 4.760E+004 2.550
 16490.0

!REF:NAROZNIK, M; NIEDZIELSKI, J. J. PHOTOCHEM. 1986, 32, 281
 IC3H7+CO<=>IC3H7CO 1.500E+011 0.000
 4810.0

!REF:CURRAN ESTIMATE
 !C3H6+HCO<=>IC3H6CHO 1.000E+011 0.000
 7800.0
 C2H3CHO+CH3<=>IC3H6CHO 1.000E+011 0.000
 7800.0

!REF:
 !IC4H8+OH<=>IC4H8OH 9.930E+011 0.000
 -960.0
 !IC4H8OH+O2<=>IO2C4H8OH 1.200E+011 0.000
 -1100.0
 !IO2C4H8OH=>CH3COCH3+CH2O+OH 1.250E+010 0.000
 18900.0
 !TC4H9O2<=>IC4H8+HO2 7.612E+042 -9.410
 41490.0

!REF:
 IC4H8OOH-TO2<=>IC4KETIT+OH 4.000E+011 0.000
 31500.0
 !REF:ANALOGY TO 1ST ISOMERISATION
 !REF:ANALOGY TO QOOH B-SCISSION
 !!C4H8OOH2-4<=>C4H8O1-3+OH 032114ADD
 !TIC4H7Q2-I=>TC4H7O2H-CYII+OH 2.440E+009 0.780
 18000.0
 !!C4H8OOH2-4=>OH+CH3CHO+C2H4 032114ADD
 !TC4H7O2H-CYII=>CH3COCH2+CH2O+OH 3.080E+008 1.500
 23500.0
 !!NC4KET14=>CH2CH2CHO+CH2O+OH 032414ADD

!TIC4H7Q2-I=>TC3H5OOH+CH2O+OH 42000.0	1.500E+016	0.000
!!PC4H9O2H<=>PC4H9O+OH 032414ADD !TC3H5OOH=>CH3COCH2+OH 42500.0	1.500E+016	0.000
!REF:CURRAN ESTIMATE !IC4H7OOH+HO2<=>TIC4H7Q2-I 10600.0	1.000E+011	0.000
!REF: IC4H8OOH-TO2<=>TIC4H7Q2-I 34500.0	6.000E+011	0.000
!REF:CURRAN ESTIMATE CH2O2H<=>CH2O+OH 1500.0	9.000E+014	0.000
!REF: !IC4H8+HO2<=>TC4H8O2H-I 12620.0	3.970E+011	0.000
!REF:GREEN 2003 !IC4H8O2H-T<=>IC4H8O+OH 13400.0	3.090E+012	0.000
!TC4H8O2H-I<=>IC4H8O+OH 17000.0	3.980E+012	0.000
! REF: GREEN 2003 DIVIDED BY 2 IC4H8O2H-T<=>IC4H8O+OH 13400.0	1.55E+012	0.000
!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES TC3H6CHO+CH2O<=>IC3H7CHO+HCO 18190.0	2.520E+008	1.900
TC3H6CHO+IC4H8<=>IC3H7CHO+IC4H7 19840.0	4.700E+002	3.300
!REF:ANALOGY TO 1C4H8+OH IC3H6CO+OH<=>IC3H7+CO2 -1010.0	1.730E+012	0.000
!REF:CURRAN ESTIMATE TC3H6CHO+OH<=>TC3H6OHCHO 0.0	5.000E+013	0.000
!REF:!TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) C3H6OH2-1+HCO<=>TC3H6OHCHO 0.0	1.810E+013	0.000
!REF:ANALOGY WITH CH3CHOH --> CH3CHO+H. !REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13 CH3COCH3+H<=>C3H6OH2-1 9500.0	8.000E+012	0.000
C2H5CHO+H<=>C3H6OH1-2 9500.0	8.000E+012	0.000

!REF:BASED ON IC4H8+H<=>IC4H9 IC3H5OH+H<=>C3H6OH2-1 4020.0	6.250E+011	0.510
!REF:REVERSE BY ANALOGY HCO+OH --> PRODUCTS C3H5-T+OH<=>IC3H5OH 0.0	5.000E+013	0.000
!REF: TC3H6CHO+O2<=>TC3H6O2CHO 0.0	1.990E+017	-2.100
TC3H6O2CHO<=>IC3H5O2HCHO 29880.0	6.000E+011	0.000
TC3H6O2CHO<=>TC3H6O2HCO 25750.0	1.000E+011	0.000
!REF:REVERSE ANALOGY IC4H8+CH3 --> NEOC5H11.		
!REF:SLAGLE ET AL. J. PHYS. CHEM. 1991, 95 IC3H5CHO+HO2<=>IC3H5O2HCHO 10600.0	2.230E+011	0.000
!REF:!MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS. CHEM. 1990, 94, 3016 C3H6OH2-1+O2<=>CH3COCH3+HO2 5000.0	1.500E+012	0.000
C3H6OH1-2+O2<=>C2H5CHO+HO2 5000.0	1.500E+012	0.000
!REF:CURRAN ESTIMATE IC3H6CO+OH<=>C3H6OH2-1+CO -1010.0	2.000E+012	0.000
!REF:!LOHDI, Z.H.; WALKER, R.W.; J. CHEM. SOC. FARAD. 1991 87, 2361 (C3H5-A+HO2) (X 0.5) TC3H6CHO+HO2<=>IC3H7CHO+O2 1310.0	3.675E+012	0.000
!REF:CURRAN ESTIMATE TC3H6CHO+CH3<=>IC3H5CHO+CH4 -131.0	3.010E+012	-0.320
!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95 TC4H8CHO<=>IC3H5CHO+CH3 26290.0	1.000E+013	0.000
TC4H8CHO<=>IC4H8+HCO 20090.0	8.520E+012	0.000
!REF:CURRAN ESTIMATE TC4H8CHO+O2<=>O2C4H8CHO 0.0	2.000E+012	0.000
O2C4H8CHO<=>O2HC4H8CO 15360.0	2.160E+011	0.000
IC4H8O2H-T+CO<=>O2HC4H8CO 4809.0	1.500E+011	0.000
!REF:PITZ ESTIMATE		

IC4H7O+IC4H8<=>IC4H7OH+IC4H7
4000.0 2.700E+011 0.000

!REF:

IC4H6OH+HO2=>CH2CCH2OH+CH2O+OH
0.0 1.446E+013 0.000

!REF:CURRAN ESTIMATE

IC4H8+CH2CCH2OH<=>IC4H7+C3H5OH
20500.0 7.940E+011 0.000

CH2CCH2OH+H2O2<=>C3H5OH+HO2
2583.0 3.010E+009 0.000

C3H5OH+OH<=>CH2CCH2OH+H2O
5960.0 5.060E+012 0.000

C3H5OH+H<=>CH2CCH2OH+H2
5821.0 3.900E+005 2.500

C3H5OH+O2<=>CH2CCH2OH+HO2
60690.0 4.000E+013 0.000

C3H5OH+CH3<=>CH2CCH2OH+CH4
8030.0 2.400E+011 0.000

!REF:CURRAN ESTIMATE

CH2CCH2OH+CH3<=>IC4H7OH
0.0 3.000E+013 0.000

CH2CCH2OH+H<=>C3H5OH
0.0 1.000E+014 0.000

CH2CCH2OH+O2=>CH2OH+CO+CH2O
0.0 4.335E+012 0.000

CH2CCH2OH<=>C2H2+CH2OH
45110.0 2.163E+040 -8.310

!C3H5-A+C2H2<=>C*CC*CCJ
6883.4 1.000E+012 0.000

C3H5-A+C2H3=>C5H6+H+H
61137.7 1.600E+035 -14.000

C3H4-A+C3H3<=>C6H6+H
9990.4 1.400E+012 0.000

C3H3+C3H3<=>C6H5+H 2.020E+033 -6.050 15940.0

C3H3+C3H3<=>C6H6 1.640E+066 -15.902 27529.0

DUP

C3H3+C3H3<=>C6H6 1.200E+035 -7.435 5058.0

DUP

C3H3+C3H3=fulvene 7.25E+65 -16.00 25035

DUP

C3H3+C3H3=fulvene 4.19E+39 -9.00 6098

DUP

C3H5-A+C3H3=fulvene+2H 3.26E+29 -5.40 3390

fulvene=C6H6 5.62E+81 -19.40 121500

fulvene+H=C6H6+H 3.00E+12 0.50 2000

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C4H6+C2H3=>C6H6+H2+H
3240.0 5.620E+011 0.000

C4H5-N+C2H2<=>C6H6+H
5400.0 1.600E+016 -1.330

C4H5-N+C2H3<=>C6H6+H2
-3611.0 1.840E-013 7.070

C4H5-2+C2H2<=>C6H6+H 25000.0	5.000E+014	0.000
C4H5-2+C2H4<=>C5H6+CH3 25000.0	5.000E+014	0.000
C6H2+H<=>C6H3 10800.0	1.100E+030	-4.920
C6H3+H<=>C4H2+C2H2 10780.0	2.800E+023	-2.550
C6H3+H<=>L-C6H4 12120.0	3.400E+043	-9.010
C6H3+H<=>C6H2+H2 0.0	3.000E+013	0.000
C6H3+OH<=>C6H2+H2O 0.0	4.000E+012	0.000
L-C6H4+H<=>C6H5 31400.0	1.700E+078	-19.720
L-C6H4+H<=>C-C6H4+H 34500.0	1.400E+054	-11.700
L-C6H4+H<=>C6H3+H2 9240.0	1.330E+006	2.530
L-C6H4+OH<=>C6H3+H2O 430.0	3.100E+006	2.000
C-C6H4+H<=>C6H5 29500.0	2.400E+060	-13.660
C4H3-N+C2H2<=>L-C6H4+H 10600.0	2.500E+014	-0.560
C4H3-N+C2H2<=>C6H5 31300.0	9.600E+070	-17.770
C4H3-N+C2H2<=>C-C6H4+H 30100.0	6.900E+046	-10.010
!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)		
C4H3-I+CH3<=>C5H6 0.0	1.000E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C4H2+C2H<=>C6H2+H 0.0	9.600E+013	0.000
C4H2+C2H<=>C6H3 7100.0	4.500E+037	-7.680
C4H4+C2H<=>L-C6H4+H 0.0	1.200E+013	0.000
!REF:WANG ET AL. C&F, 110: 173. 1994		
C6H5+H(+M)<=>C6H6(+M) 0.0	1.000E+014	0.000
LOW/ 7000.0/	6.600E+075	-16.300
TROE/ 1.000E+000 1.000E-001 5.849E+002 6.113E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/		
!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
C6H6+O2<=>C6H5+HO2 60000.0	6.300E+013	0.000
!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)		
C6H6+O<=>C6H5O+H 4530.0	2.200E+013	0.000

!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)		
C6H6+O<=>C6H5+OH 14700.0	2.000E+013	0.000
!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
C6H6+H<=>C6H5+H2 16000.0	2.500E+014	0.000
!REF:ESTIMATED		
C6H6+CH3<=>C6H5+CH4 18920.0	7.320E+012	0.000
!REF:ESTIMATED		
C6H6+HO2<=>C6H5+H2O2 28900.0	5.500E+012	0.000
!REF:CHEN&BOZ J. PHYS. CHEM. A 108: 4632 - 4652 2004		
C6H6+OH<=>C6H5+H2O -301.0	1.200E+000	4.100
!REF:TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI J. PHYS. CHEM. A, 2006, 110 (15), 5081-5090		
C6H6+OH<=>C6H5OH+H 5590.0	1.320E+002	3.250
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C6H5=>H+C4H2+C2H2 77294.0	4.300E+012	0.620
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C6H5+CH2O<=>C6H6+HCO 38.0	8.550E+004	2.190
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C6H5+HCO<=>C6H6+CO 38.0	8.550E+004	2.190
!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5+HO2<=>C6H5O+OH 0.0	5.000E+012	0.000
!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.		
C6H5+O2<=>C6H5O+O 6120.0	2.600E+013	0.000
!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.		
C6H5+O2<=>O-C6H4O2+H 8980.0	3.000E+013	0.000
!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575		

C6H5+O2<=>C6H5OO -711.0	1.860E+013	-0.220
!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575		
C6H5OO<=>C6H5O+O 38536.0	1.270E+015	-0.246
!REF:WKM ESTIMATED		
C6H5O+OH<=>C6H5OOH 0.0	2.000E+013	0.000
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C6H5OO+C6H5OH<=>C6H5OOH+C6H5O 14000.0	1.330E+011	0.000
!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+O2<=>C6H5O+HO2 38800.0	1.000E+013	0.000
C6H5OH+O<=>OC6H4OH+H 3400.0	1.600E+013	0.000
C6H5OH+H<=>C6H5O+H2 12400.0	1.200E+014	0.000
C6H5OH+O<=>C6H5O+OH 2900.0	1.300E+013	0.000
C6H5OH+OH<=>C6H5O+H2O -960.0	1.400E+008	1.400
C6H5OH+HO2<=>C6H5O+H2O2 10000.0	1.000E+012	0.000
C6H5OH+CH3<=>C6H5O+CH4 7700.0	1.800E+011	0.000
C6H5OH+C6H5<=>C6H5O+C6H6 4400.0	4.900E+012	0.000
C6H5OH+C3H5-A<=>C6H5O+C3H6 9400.0	4.900E+011	0.000
C6H5OH+C4H5-I<=>C6H5O+C4H6 9400.0	4.900E+011	0.000
C6H5OH+H<=>C6H4OH+H2 16000.0	1.700E+014	0.000
C6H5OH+O<=>C6H4OH+OH 14700.0	2.000E+013	0.000
C6H5OH+OH<=>C6H4OH+H2O 4600.0	1.400E+013	0.000
C6H5OH+HO2<=>C6H4OH+H2O2 28900.0	4.000E+011	0.000
C6H5OH+CH3<=>C6H4OH+CH4 15000.0	2.000E+012	0.000
C6H4OH+O2<=>OC6H4OH+O 6100.0	2.100E+013	0.000
C6H4OH+H<=>C6H5OH 0.0	1.000E+014	0.000
OC6H4OH<=>C5H4OH+CO 43800.0	7.400E+011	0.000
!REF:WKM REDUCED FROM 2.5E+14		
!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
C6H5O+H(+M)<=>C6H5OH(+M) 0.0	2.000E+014	0.000

LOW/ 13880.0/ TROE/ 4.300E-002 3.042E+002 6.000E+004 5.896E+003/	1.000E+094	-21.840
!REF:XU AND LIN J PHYS CHEM 110 1672-1677 2006		
!REF:WKM A FACTOR *0.5 TO FIT PYROLYSIS DATA		
C6H5OH<=>C5H6+CO 74115.0	4.310E+015	-0.610
!REF:BAULCH AND COBOS		
!REF:EVALUATED KINETIC DATA FOR COMBUSTION MODELLING J. PHYS. CHEM. REF. DATA 21, 411-429 (1992)		
!REF:WKM A FACTOR REDUCED FROM 2.5E+11 TO 2.0E+11 TO FIT DATA BENZENE FLOW REACTOR DATA (LOVELL)		
C6H5O<=>CO+C5H5 43900.0	2.000E+011	0.000
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C6H5O+H<=>CO+C5H6 0.0	1.000E+013	0.000
C6H5O+O<=>C5H5+CO2 0.0	1.000E+013	0.000
C6H5O+O<=>OC6H4OH 800.0	2.600E+010	0.470
!REF:WKM		
!REF:ESTIMATED TO IMPROVE AGREEMENT WITH		
!REF:TOLUENE FLOW REACTOR DATA. PATHWAY TO FORM		
!REF:PARABENZOQUINONE REMOVED AS IT CAUSED IT TO BUILD		
!REF:UP AND IT IS NOT SEEN IN THE EXPERIMENT		
C6H5O+HO2<=>O-OC6H5OJ+OH 0.0	2.000E+012	0.000
!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38: 250-275, 2006		
P-C6H4O2+H<=>P-OC6H5OJ 9740.0	4.000E+012	0.000
!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38: 250-275, 2006		
O-C6H4O2+H<=>O-OC6H5OJ 6960.0	4.000E+012	0.000
!REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998		
C6H5O+O<=>P-C6H4O2+H 0.0	4.250E+013	0.000
C6H5O+O<=>O-C6H4O2+H 0.0	8.500E+013	0.000
O-C6H4O2<=>C5H4O+CO 40000.0	1.000E+012	0.000
P-C6H4O2<=>C5H4O+CO 59000.0	3.700E+011	0.000

P-C6H4O2+H<=>C5H5O+CO 4700.0	2.500E+013	0.000
P-C6H4O2+H<=>P-C6H3O2+H2 8100.0	2.000E+012	0.000
P-C6H4O2+O<=>P-C6H3O2+OH 14700.0	1.400E+013	0.000
P-C6H4O2+OH<=>P-C6H3O2+H2O 4000.0	1.000E+006	2.000
P-C6H3O2+H<=>P-C6H4O2 0.0	1.000E+014	0.000
P-C6H3O2+H<=>2C2H2+2CO 0.0	1.000E+014	0.000
P-C6H3O2+O=>C2H2+HCCO+2CO 0.0	1.000E+014	0.000

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007

P-C6H4O2+O=>2CO+C2H2+CH2CO 5000.0	3.000E+013	0.000
C5H5+H(+M)<=>C5H6(+M) 0.0	2.600E+014	0.000
LOW/ 12994.0/	4.400E+080	-18.280
TROE/ 6.800E-002 4.007E+002 4.136E+003 5.502E+003/ CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/		

!REF:MACKIE ET AL. PHYS CHEM CHEM PHYS 3 2467 2001

!REF:TROE FIT ADDED BY WKM (CHEMDIS)

C5H6(+M)<=>C3H4-A+C2H2(+M) 104000.0	3.800E+017	0.000
LOW/ 126321.5/	1.000E+098	-22.250
TROE/ 1.441E-001 5.358E+000 3.284E+003 6.710E+009/ CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/		

!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+O2<=>C5H5+HO2 37150.0	4.000E+013	0.000
C5H6+HO2<=>C5H5+H2O2 12900.0	1.100E+004	2.600
C5H6+OH<=>C5H5+H2O 0.0	3.080E+006	2.000

!REF:ROY AND FRANK, 21ST INTERNATIONAL SYMPOSIUM ON SHOCKWAVES, 1997 PPER 1560

C5H6+H<=>C5H5+H2 3500.0	7.200E+013	0.000
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!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

!C5H6+H<=>C2H2+C3H5-A 32890.0	1.548E+037	-6.180
C5H6+O<=>C5H5+OH 1100.0	4.800E+004	2.710
C5H6+C2H3<=>C5H5+C2H4 0.0	1.200E-001	4.000

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161

C5H6+C6H5O<=>C5H5+C6H5OH 8000.0	3.160E+011	0.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+CH3<=>C5H5+CH4 0.0	1.800E-001	4.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+C6H5<=>C5H5+C6H6 0.0	1.000E-001	4.000
!REF:ON OTHER CONDITIONS.		
C5H6+C5H5<=>C6H6+C4H5-N 0.0	5.000E+009	0.000
!REF:LIN J COMPUT CHEM 21 415-425 2000		
C5H5<=>C3H3+C2H2 124900.0	1.980E+068	-15.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H5+O<=>C4H5-N+CO 440.0	3.200E+013	-0.170
C5H5+O<=>C5H4O+H 20.0	5.800E+013	-0.020
C5H5+OH<=>C5H5OH -2730.0	6.500E+014	-0.850
DUP		
C5H5+OH<=>C5H5OH 18730.0	1.100E+043	-8.760
DUP		
C5H5+OH<=>C5H5OH 33450.0	1.100E+059	-13.080
DUP		
C5H5+OH<=>C5H4OH+H 48350.0	3.500E+057	-12.180
!REF:RISTORI ET AL. COMBUST. SCI. AND TECH 2001. VOL. 167. PP. 223-256		
C5H5+OH<=>C4H6+CO 4500.0	4.000E+014	0.000
C5H5+HO2<=>C5H5O+OH 11650.0	6.300E+029	-4.690
!REF:WKM REDUCED BY 50% TO PROVIDE		
!REF:AGREEMENT WITH C5H6 SHOCK TUBE DATA		
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H5+O2<=>C4H4O+HCO 10970.0	6.000E+018	-2.480
!REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000		
C4H4O+H<=>C3H5-A+CO 2740.0	6.600E+013	-0.020
DUP		
C4H4O+H<=>C3H5-A+CO 1300.0	5.900E+006	2.000
DUP		

C4H4O+O<=>CH2CHO+HCCO 3.000E+008 1.450
-860.0
C4H4O+OH<=>C3H5-A+CO2 3.000E+012 0.000
0.0

!REF:LIN J COMPUT CHEM 21 415-425 2000
C3H3+C2H2<=>C#CC*CCJ 4.110E+072 -18.200
45400.0
C#CC*CCJ<=>C5H5 8.000E+013 0.000
34058.3
C#CC*CCJ+H<=>C5H6 1.000E+014 0.000
0.0

!REF:LINDSTEDT C&F 99:551-561 (1994)
C#CC*CCJ+H<=>C5H6-L 1.000E+010 0.000
0.0
C5H6-L+O<=>C#CC*CCJ+OH 1.000E+010 0.000
0.0
C5H6-L+OH<=>C#CC*CCJ+H2O 1.000E+010 0.000
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C5H5OH+H<=>C5H4OH+H2 3.200E+012 0.000
0.0
C5H5OH+H<=>C5H5O+H2 4.000E+013 0.000
6094.0
C5H5OH+OH<=>C5H4OH+H2O 5.500E+012 0.000
1731.0
C5H5OH+OH<=>C5H5O+H2O 1.000E+013 0.000
1697.0
C5H5OH+O<=>C5H4OH+OH 4.700E+011 0.000
0.0
C5H5OH+O<=>C5H5O+OH 1.000E+013 0.000
4683.0
C5H5OH+HO2<=>C5H4OH+H2O2 3.600E+003 2.550
10531.0
C5H5OH+HO2<=>C5H5O+H2O2 1.000E+013 0.000
15800.0
C5H5O<=>C5H4O+H 2.900E+032 -6.500
21220.0
C5H5O<=>C4H5-N+CO 1.100E+079 -19.620
66250.0
C5H5O<=>CJ*CC*CC*O 2.000E+013 0.000
14338.0

!REF:ESTIMATED FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE C&F 114: 149-
177 (1998)
CJ*CC*CC*O<=>C*CC*CCJ*O 4.300E+011 -1.050
4118.0

!REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO
C4H5-N+CO<=>C*CC*CCJ*O 1.510E+011 0.000
4810.0

!REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-
418

CJ*CC*CC*O<=>C2H2+CJ*CC*O 43710.0	3.000E+013	0.000
CJ*CC*O<=>C2H3CO 32100.0	1.400E+009	0.980
C2H2+HCO<=>CJ*CC*O 7755.0	7.770E+006	1.410
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
C5H4OH+H<=>C5H5OH 0.0	1.000E+014	0.000
C5H4OH+H<=>C5H4O+H2 54000.0	2.100E+013	0.000
C5H4OH+O2<=>C5H4O+HO2 5000.0	3.000E+013	0.000
!REF:WANG AND BREZINSKY J PHYS CHEM A 102: 1530 1998		
C5H4O=>CO+C2H2+C2H2 68500.0	5.700E+032	-6.760
DUP C5H4O=>CO+C2H2+C2H2 98700.0	6.200E+041	-7.870
DUP		
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H4O+H<=>C4H5-N+CO 40810.0	2.100E+061	-13.270
!REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.		
C5H4O+O<=>C4H4+CO2 2000.0	1.000E+013	0.000
C5H4O+H<=>C5H3O+H2 8100.0	2.000E+012	0.000
C5H4O+O<=>C5H3O+OH 1470.0	1.400E+013	0.000
C5H4O+OH<=>C5H3O+H2O 1450.0	1.100E+008	1.420
C5H3O+H<=>C5H4O 0.0	1.000E+014	0.000
!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007		
C5H3O+O2=>CO2+C2H2+HCCO 38180.0	9.700E+058	-13.470
C5H3O=>C2H2+CO+C2H 51000.0	2.000E+013	0.000
!REF:ARENDS ET AL. J PHYS CHEM 97: 7914 1993		
C5H7<=>C*CCJC*C 39500.0	3.200E+015	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
C5H7+H<=>C5H6+H2 0.0	3.600E+012	0.000
C5H7+O<=>C5H6+OH 0.0	1.000E+013	0.000

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C5H7+OH<=>C5H6+H2O 2.400E+013 0.000
0.0
C5H7+O2<=>OC5H7O 8.900E+024 -3.800
20000.0

!REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998
C5H6+H<=>C5H7 2.400E+073 -17.850
31500.0
C5H6+H<=>C*CCJC*C 1.100E+014 -0.160
3100.0
C5H6+O<=>C5H5O+H 8.900E+012 -0.150
590.0
DUP
C5H6+O<=>C5H5O+H 5.600E+012 -0.060
200.0
DUP
C5H6+OH<=>C*CCJC*COH 1.100E+013 -0.070
870.0
C5H6+HO2<=>C5H7+O2 1.300E+015 -1.070
9530.0
C5H6+HCO<=>C5H5+CH2O 1.080E+008 1.900
16000.0
C5H6+C2H3<=>C6H6+CH3 2.100E+067 -16.080
42460.0

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
C5H6+C4H5-I<=>C5H5+C4H6 6.000E+012 0.000
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
!C*CCJC*C<=>C*CC*CCJ 5.400E+011 -0.700
60.0
C*CC*CCJ+H<=>C*CC*CC 2.300E+020 -1.600
3020.0
C*CC*CC+H<=>C4H6+CH3 5.200E+071 -16.380
51000.0

!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
C*CC*CC+OH<=>C*CC*CCJ+H2O 7.000E+006 2.000
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C*CCJC*C+O2<=>C2H3CHO+CH2CHO 1.200E+036 -7.250
33600.0
C*CC*CCJ+H<=>C4H5-N+CH3 2.900E+026 -2.180
36770.0

!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
C*CCJC*C+O<=>C2H3CHO+C2H3 2.000E+014 0.000
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
 $C^*CC^*CCJ+OH \rightleftharpoons C^*CC^*CCOH$ 1.500E+013 0.000
0.0
 $C^*CC^*CCJ+O_2 \rightleftharpoons C^*CC^*CCJ^*O+CH_2O$ 8.200E+010 0.180
9140.0
 $C^*CC^*CCOH+H \rightleftharpoons C_4H_6+CH_2OH$ 2.500E+034 -6.120
16250.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
 $OC_5H_7O+O_2 \rightleftharpoons OC_4H_6O+HOCO$ 6.300E+005 -7.250
33600.0
 $C^*CC^*CCJ^*COH+O_2 \rightleftharpoons HOC^*CC^*O+CH_2CHO$ 1.200E+036 -7.250
33600.0
 $HOC^*CC^*O+OH \rightleftharpoons HOC^*CC^*O+H_2O$ 2.690E+010 0.760
-340.0
 $HOC^*CC^*O+HO_2 \rightleftharpoons HOC^*CC^*O+H_2O_2$ 1.000E+012 0.000
11920.0
 $HOC^*CC^*O+CH_3 \rightleftharpoons HOC^*CC^*O+CH_4$ 3.980E+012 0.000
8700.0
 $HOC^*CC^*O+O \rightleftharpoons HOC^*CC^*O+OH$ 7.180E+012 0.000
1389.0
 $HOC^*CC^*O+O_2 \rightleftharpoons HOC^*CC^*O+HO_2$ 2.000E+013 0.000
40700.0
 $HOC^*CC^*O+H \rightleftharpoons HOC^*CC^*O+H_2$ 2.600E+012 0.000
2600.0

!REF:WKM ANALOGY TO $C_2H_5+CO \rightleftharpoons C_2H_5CO$
 $C_2H_2OH+CO \rightleftharpoons HOC^*CC^*O$ 1.510E+011 0.000
4810.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
 $OC_4H_6O+H \rightleftharpoons OC_4H_5O+H_2$ 2.300E+010 1.050
3279.0
 $OC_4H_6O+OH \rightleftharpoons OC_4H_5O+H_2O$ 3.500E+009 1.180
-447.0
 $OC_4H_5O+O_2 \rightleftharpoons O_2CCHOOJ+C_2H_4$ 1.600E+045 -9.920
20670.0
 $O_2CCHOOJ \rightleftharpoons HOCO+CO_2$ 3.000E+013 0.000
4000.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

$C^*CC^*CCJ^*O \rightleftharpoons C_3H_5-A+CO$ 6.100E+005 0.920
-1120.0
 $C^*CC^*CCJ^*O+O_2 \rightleftharpoons C_2H_3CHO+HOCO$ 1.200E+036 -7.250
33600.0

!REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013

$HOCO \rightleftharpoons CO+OH$ 6.300E+032 -5.960
32470.0
PLOG/ 0.0010 1.550E-008 2.930 8768.0/
PLOG/ 0.0030 1.770E+003 0.340 18076.0/
PLOG/ 0.0296 2.020E+013 -1.870 22755.0/
PLOG/ 0.0987 1.680E+018 -3.050 24323.0/

PLOG/	0.2961	2.500E+024	-4.630	27067.0/		
PLOG/	0.9869	4.540E+026	-5.120	27572.0/		
PLOG/	2.9607	7.120E+028	-5.600	28535.0/		
PLOG/	9.8690	5.480E+029	-5.700	28899.0/		
PLOG/	29.6070	9.890E+031	-6.190	30518.0/		
PLOG/	98.6900	5.740E+033	-6.530	32068.0/		
PLOG/	296.0700	2.610E+033	-6.290	32231.0/		
PLOG/	986.9000	6.300E+032	-5.960	32470.0/		
HOCO<=>CO2+H				1.897E+038		-8.047
34240.0						
PLOG/	0.0010	4.758E+018	-3.817	17676.0/		
PLOG/	0.0030	2.225E+020	-4.149	19037.0/		
PLOG/	0.0099	7.564E+021	-4.434	20325.0/		
PLOG/	0.0296	9.107E+024	-5.189	22419.0/		
PLOG/	0.0987	3.144E+029	-6.376	25233.0/		
PLOG/	0.2961	1.150E+032	-7.037	26662.0/		
PLOG/	0.9869	1.069E+036	-8.107	29064.0/		
PLOG/	2.9607	2.438E+036	-8.153	29336.0/		
PLOG/	9.8690	6.663E+035	-7.919	29217.0/		
PLOG/	29.6070	1.723E+038	-8.506	31273.0/		
PLOG/	98.6900	3.007E+041	-9.290	33966.0/		
PLOG/	296.0700	6.767E+036	-7.832	31613.0/		
PLOG/	986.9000	1.897E+038	-8.047	34240.0/		
!C6H10+H<=>C6H9-A+H2				6.752E+005		2.360
207.0						
!C6H10+CH3<=>C6H9-A+CH4				7.380E+000		3.310
4002.0						
C6H10+O<=>C6H9-A+OH				1.320E+006		2.430
1210.0						
!C6H10+OH<=>C6H9-A+H2O				5.528E+004		2.640
-1919.0						
!C4H6+C2H3<=>C6H9-A				8.800E+005		2.500
6130.0						
!REF: FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776						
C6H10<=>C3H5-A+C3H5-A				4.900E+022		-2.060
63355.5						
PLOG/	1.0000	5.070E+047	-9.700	72680.0/		
PLOG/	4.0000	4.220E+039	-7.300	69390.0/		
PLOG/	10.0000	2.120E+035	-6.000	67620.0/		
C3H5-A+C3H5-A<=>C3H4-A+C3H6				9.550E+040		-9.300
12470.0						
PLOG/	1.0000	4.770E+040	-9.300	12470.0/		
PLOG/	4.0000	3.970E+032	-6.800	9180.0/		
PLOG/	10.0000	1.460E+028	-5.500	7410.0/		
C6H10+O2<=>C6H9-A+HO2				4.000E+014		0.000
38890.0						
C6H10+H=>C3H4-A+C3H5-A+H2				1.000E+012		0.000
0.0						
C6H10+H<=>C3H5-A+C3H6				1.000E+013		0.000
0.0						

!!!!!!!!!!!!!!!!!!!!DME SUBMECHANISM

!REF:R. SIVARAMAKRISHNAN, J.V. MICHAEL, A.F. WAGNER, R. DAWES, A.W. JASPER, L.B. HARDING, Y. GEORGIEVSKII, S.J. KLIPPENSTEIN, COMBUSTION AND FLAME, 158 (2011) 618-632.

CH3OCH3 (+M) <=> CH3+CH3O (+M)	2.330E+019	-0.661
84139.0		
LOW/	1.720E+059	-11.400
93295.6/		
TROE/ 1.000E+000 1.000E-030 8.80E+002/		
H2/ 3.00/ CO/ 2.25/ CO2/ 3.00/ N2/ 1.50/ H2O/ 9.00/ CH3OCH3/ 5.00/ CH4/		
3.00/ C2H6/ 4.50/		
!REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.		
CH3OCH3+OH<=>CH3OCH2+H2O	9.350E+005	2.290 -780.7
!REF:CURRAN, FIT TO NIST DATABASE		
CH3OCH3+H<=>CH3OCH2+H2	7.721E+006	2.090
3384.0		
!REF:CURRAN 08 NIST FIT		
CH3OCH3+O<=>CH3OCH2+OH	7.750E+008	1.360
2250.0		
!REF:J. MENDES, C.-W. ZHOU, H.J. CURRAN, THE JOURNAL OF PHYSICAL CHEMISTRY A, 118 (2014) 1300-1308.		
CH3OCH3+HO2<=>CH3OCH2+H2O2	3.170E-003	4.640
10556.0		
CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H	1.268E-003	4.640
10556.0		
!REF:R.S. TRANTER, P.T. LYNCH, C.J. ANNESLEY, THE JOURNAL OF PHYSICAL CHEMISTRY A, 116 (2012) 7287-7292. (A-FACTOR - 3.0)		
CH3OCH3+CH3<=>CH3OCH2+CH4	7.020E+000	3.780
9687.1		
!REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.		
CH3OCH3+O2<=>CH3OCH2+HO2	4.100E+013	0.000
44910.0		
!REF:ESTIMATE, S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.		
CH3OCH3+CH3O<=>CH3OCH2+CH3OH	6.020E+011	0.000
4074.0		
!REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.		
CH3OCH3+CH3OCH2O2<=>CH3OCH2+CH3OCH2O2H	5.000E+012	0.000
17690.0		
CH3OCH3+O2CHO<=>CH3OCH2+HO2CHO	4.425E+004	2.600
13910.0		
CH3OCH3+OCHO<=>CH3OCH2+HOCHO	1.000E+013	0.000
17690.0		
!REF:KPS RRKM/ME CALC, AN IGNITION DELAY AND KINETIC MODELING STUDY OF METHANE, DIMETHYL ETHER, AND THEIR MIXTURES AT HIGH PRESSURES. CNF 2014		
CH3OCH2<=>CH3+CH2O	8.03E+12	0.440284 26490.7
PLOG/ 1.00E-02	7.494E+23	-4.5152 25236.1/
PLOG/ 1.00E-01	6.921E+28	-5.7271 27494.9/
PLOG/ 1.00E+00	4.229E+29	-5.6103 28898.3/
PLOG/ 1.00E+01	6.608E+27	-4.7073 29735.2/

PLOG/ 1.00E+02 2.659E+29 -4.9358 31785.5/

!REF:QRRK CALC. BASED ON: T. YAMADA, J.W. BOZZELLI, T.H. LAY,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452.
!REF:R+O2 HPL=S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

CH3OCH2+O2<=>CH3OCH2O2 1.0 1.0 1.0

PLOG/ 1.000E-003 1.120E+018 -3.37 -4294./

PLOG/ 1.000E-002 1.330E+021 -3.95 -2615./

PLOG/ 1.000E+000 1.130E+028 -5.24 4088./

PLOG/ 2.000E+000 3.910E+027 -5.00 4512./

PLOG/ 1.000E+001 2.750E+024 -3.87 4290./

PLOG/ 2.000E+001 2.970E+022 -3.23 3781./

PLOG/ 5.000E+001 5.190E+019 -2.35 2908./

PLOG/ 1.000E+002 5.430E+017 -1.73 2210./

CH3OCH2+O2<=>CH2OCH2O2H 1.0 1.0 1.0

PLOG/ 1.000E-003 5.080E+020 -4.39 469./

PLOG/ 1.000E-002 5.470E+023 -4.96 2183./

PLOG/ 1.000E+000 2.810E+028 -5.63 7848./

PLOG/ 2.000E+000 5.190E+027 -5.33 8144./

PLOG/ 1.000E+001 9.670E+024 -4.36 8417./

PLOG/ 2.000E+001 4.080E+023 -3.90 8494./

PLOG/ 5.000E+001 5.080E+021 -3.28 8585./

PLOG/ 1.000E+002 1.620E+020 -2.81 8619./

CH3OCH2+O2<=>CH2O+CH2O+OH 1.0 1.0 1.0

PLOG/ 1.000E-003 8.010E+021 -3.18 3067./

PLOG/ 1.000E-002 1.730E+023 -3.55 4050./

PLOG/ 1.000E+000 2.040E+031 -5.76 11594./

PLOG/ 2.000E+000 5.990E+031 -5.87 12710./

PLOG/ 1.000E+001 9.390E+030 -5.59 14517./

PLOG/ 2.000E+001 1.090E+030 -5.30 15051./

PLOG/ 5.000E+001 3.580E+028 -4.88 15664./

PLOG/ 1.000E+002 2.410E+027 -4.55 16107./

CH3OCH2O2<=>CH2OCH2O2H 1.0 1.0 1.0

PLOG/ 1.000E-003 1.940E+029 -6.99 22446./

PLOG/ 1.000E-002 4.070E+027 -6.16 21619./

PLOG/ 1.000E+000 2.520E+025 -4.76 22691./

PLOG/ 2.000E+000 5.970E+024 -4.48 22868./

PLOG/ 1.000E+001 4.440E+021 -3.38 22386./

PLOG/ 2.000E+001 4.520E+019 -2.74 21803./

PLOG/ 5.000E+001 5.720E+016 -1.82 20829./

PLOG/ 1.000E+002 3.700E+014 -1.13 20034./

CH3OCH2O2<=>CH2O+CH2O+OH 1.0 1.0 1.0

PLOG/ 1.000E-003 2.060E+036 -8.32 33415./

PLOG/ 1.000E-002 2.070E+039 -8.86 35842./

PLOG/ 1.000E+000 1.120E+040 -8.42 39835./

PLOG/ 2.000E+000 9.720E+038 -8.04 39923./

PLOG/ 1.000E+001 6.280E+035 -6.97 39900./

PLOG/ 2.000E+001 1.600E+034 -6.46 39850./

PLOG/ 5.000E+001 8.320E+031 -5.75 39719./

PLOG/ 1.000E+002 1.220E+030 -5.20 39549./

CH2OCH2O2H<=>CH2O+CH2O+OH 1.0 1.0 1.0

PLOG/ 1.000E-003 1.660E+023 -4.53 22243./

PLOG/ 1.000E-002 5.300E+025 -4.93 24158./

PLOG/ 1.000E+000 7.810E+022 -3.50 23156./

PLOG/ 2.000E+000 4.980E+022 -3.35 23062./

PLOG/ 1.000E+001 8.460E+022 -3.22 23559./

PLOG/ 2.000E+001 9.090E+022 -3.14 23899./

PLOG/ 5.000E+001 4.590E+022 -2.94 24262./
PLOG/ 1.000E+002 1.400E+022 -2.72 24407./

!REF:QRRK CALC. BASED ON: T. YAMADA, J.W. BOZZELLI, T.H. LAY,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452.
!REF:R+O2 HPL=S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

CH2OCH2O2H+O2<=>O2CH2OCH2O2H 1.0 1.0 1.0
PLOG/ 1.000E-003 9.420E+012 -1.68 -4998./
PLOG/ 1.000E-002 8.160E+016 -2.50 -2753./
PLOG/ 1.000E+000 1.060E+022 -3.30 3389./
PLOG/ 2.000E+000 3.480E+020 -2.79 3131./
PLOG/ 1.000E+001 2.860E+016 -1.48 1873./
PLOG/ 2.000E+001 8.550E+014 -1.01 1312./
PLOG/ 5.000E+001 2.680E+013 -0.54 727./
PLOG/ 1.000E+002 4.870E+012 -0.32 428./
CH2OCH2O2H+O2<=>HO2CH2OCHO+OH 1.0 1.0 1.0
PLOG/ 1.000E-003 5.900E+020 -2.88 3234./
PLOG/ 1.000E-002 2.060E+023 -3.59 5116./
PLOG/ 1.000E+000 4.450E+029 -5.29 12791./
PLOG/ 2.000E+000 2.440E+028 -4.92 12891./
PLOG/ 1.000E+001 9.420E+023 -3.68 12049./
PLOG/ 2.000E+001 1.040E+022 -3.16 11505./
PLOG/ 5.000E+001 6.950E+019 -2.60 10861./
PLOG/ 1.000E+002 3.960E+018 -2.31 10500./
O2CH2OCH2O2H<=>HO2CH2OCHO+OH 1.0 1.0 1.0
PLOG/ 1.000E-003 9.050E+023 -4.88 18805./
PLOG/ 1.000E-002 6.840E+026 -5.32 22533./
PLOG/ 1.000E+000 5.070E+016 -1.81 21175./
PLOG/ 2.000E+000 2.660E+014 -1.11 20310./
PLOG/ 1.000E+001 1.690E+010 0.18 18604./
PLOG/ 2.000E+001 1.110E+009 0.54 18100./
PLOG/ 5.000E+001 1.070E+008 0.84 17661./
PLOG/ 1.000E+002 3.860E+007 0.98 17467./

!REF:K.A. SAHETCHIAN, R. RIGNY, J. TARDIEU DE MALEISSYE, L. BATT, M.
ANWAR KHAN, S. MATHEWS, SYMPOSIUM (INTERNATIONAL) ON COMBUSTION, 24
(1992) 637-643. A-FACTOR X5.

HO2CH2OCHO<=>OCH2OCHO+OH 5.000E+016 0.000
43000.0

!REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF
CHEMICAL KINETICS, 32 (2000) 713-740.

CH3OCH2+CH3O<=>CH3OCH3+CH2O 2.410E+013 0.000
0.0
CH3OCH2+CH2O<=>CH3OCH3+HCO 5.490E+003 2.800
5862.0
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO 1.260E+012 0.000
8499.0

!REF:!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

!REF:!1/ 2 CH3O2+CH2O<=>CH3O2H+HCO
CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO 1.000E+012 0.000
11660.0

!REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF
CHEMICAL KINETICS, 32 (2000) 713-740.

CH2+C3H6<=>CCYCCC			1.000E+011	0.000
0.0				
PLOG/	0.0100	6.16E+40	-10.5	5428.1/
PLOG/	0.1000	6.93E+41	-10.3	6188.9/
PLOG/	1.0000	1.81E+37	-8.55	5521/
PLOG/	10.0000	4.26E+37	-8.32	4770.2/
PLOG/	100.0000	4.68E+35	-7.37	4689.1/
DUP				

CH2+C3H6<=>IC4H8			1.000E+011	0.000
0.0				
PLOG/	0.0100	4.82E+57	-14.34	17091/
PLOG/	0.1000	3.84E+59	-14.36	18427/
PLOG/	1.0000	2.13E+58	-13.45	20355/
PLOG/	10.0000	8.48E+52	-11.63	20677/
PLOG/	100.0000	6.07E+47	-9.85	22055/
DUP				

CH2+C3H6<=>IC4H8			1.000E+011	0.000
0.0				
PLOG/	0.0100	1.15E+45	-11.13	6145.2/
PLOG/	0.1000	1.83E+45	-10.68	6638.5/
PLOG/	1.0000	1.30E+40	-8.7703	5863.8/
PLOG/	10.0000	2.27E+32	-6.1375	4317.9/
PLOG/	100.0000	1.28E+24	-3.4904	2529.9/
DUP				

CH2+C3H6<=>IC4H7+H			1.000E+011	0.000
0.0				
PLOG/	0.0100	8.20E+19	-2.06	1145.2/
PLOG/	0.1000	2.27E+21	-2.44	2648.4/
PLOG/	1.0000	4.44E+35	-6.55	13894/
PLOG/	10.0000	1.18E+28	-4.09	14013/
PLOG/	100.0000	6.51E+26	-3.58	18927/
DUP				

CH2+C3H6<=>IC4H7+H			1.000E+011	0.000
0.0				
PLOG/	0.0100	1.08E+07	1.62	-3174.6/
PLOG/	0.1000	1.37E+05	2.15	-3799.2/
PLOG/	1.0000	3.89E+14	-0.42	1237.6/
PLOG/	10.0000	2.45E+10	0.67	750.93/
PLOG/	100.0000	1.81E+02	2.97	-746.03/
DUP				

CH2+C3H6<=>C3H5-T+CH3			1.000E+011	0.000
0.0				
PLOG/	0.0100	1.77E+19	-1.94	6786.8/
PLOG/	0.1000	1.68E+19	-1.8	4310.4/
PLOG/	1.0000	4.16E+24	-3.19	9758.5/
PLOG/	10.0000	7.89E+24	-3.07	13894/
PLOG/	100.0000	7.36E+29	-4.28	23849/
DUP				

CH2+C3H6<=>C3H5-T+CH3			1.000E+011	0.000
0.0				
PLOG/	0.0100	4.30E+12	0.19	-110.41/
PLOG/	0.1000	2.26E+11	0.54	47.81/
PLOG/	1.0000	4.92E+09	1.02	599.77/
PLOG/	10.0000	1.47E+08	1.33	1228.4/
PLOG/	100.0000	8.11E+10	0.55	5506.5/

DUP

C3H5-T+CH3<=>IC4H8 1.000E+011 0.000
0.0
PLOG/ 0.0100 1.93E+61 -14.91 19559/
PLOG/ 0.1000 7.49E+58 -13.81 20442/
PLOG/ 1.0000 9.74E+55 -12.62 21930/
PLOG/ 10.0000 7.70E+50 -10.88 22198/
PLOG/ 100.0000 2.07E+48 -9.9 24315/

DUP

C3H5-T+CH3<=>IC4H8 1.000E+011 0.000
0.0
PLOG/ 0.0100 3.78E+46 -11.15 7331.5/
PLOG/ 0.1000 2.86E+40 -8.97 6234.4/
PLOG/ 1.0000 7.24E+33 -6.71 4848.4/
PLOG/ 10.0000 2.28E+27 -4.53 3329.3/
PLOG/ 100.0000 5.40E+23 -3.31 2521.8/

DUP

C3H5-T+CH3<=>IC4H7+H 1.000E+011 0.000
0.0
PLOG/ 0.0100 4.12E+29 -4.95 7995.8/
PLOG/ 0.1000 4.86E+30 -5.03 11287/
PLOG/ 1.0000 5.30E+29 -4.57 14443/
PLOG/ 10.0000 1.32E+30 -4.54 19255/
PLOG/ 100.0000 5.16E+28 -4.03 23821/

DUP

C3H5-T+CH3<=>IC4H7+H 1.000E+011 0.000
0.0
PLOG/ 0.0100 5.73E+15 -0.77 1195.9/
PLOG/ 0.1000 2.06E+13 -0.074 1428.7/
PLOG/ 1.0000 4.48E+10 0.6 1421.6/
PLOG/ 10.0000 4.10E+06 1.71 1056.9/
PLOG/ 100.0000 1.37E-01 3.91 -353.55/

DUP

IC4H7+H<=>IC4H8 1.000E+011 0.000
0.0
PLOG/ 0.0100 2.00E+64 -15.02 23890/
PLOG/ 0.1000 1.40E+61 -13.84 24846/
PLOG/ 1.0000 1.00E+58 -12.7 25947 /
PLOG/ 10.0000 1.68E+53 -11.13 25910/
PLOG/ 100.0000 6.89E+44 -8.62 22842 /

DUP

IC4H7+H<=>IC4H8 1.000E+011 0.000
0.0
PLOG/ 0.0100 1.85E+40 -8.58 6466.1/
PLOG/ 0.1000 3.37E+34 -6.64 5193/
PLOG/ 1.0000 9.06E+29 -5.1 4171.5/
PLOG/ 10.0000 4.77E+25 -3.68 3143.1/
PLOG/ 100.0000 1.10E+21 -2.16 1916.5/

DUP

IC4H8<=>CCYCCC 1.000E+011 0.000 0.0
PLOG/ 0.0100 1.26E+64 -15.57 95033/
PLOG/ 0.1000 3.94E+67 -16.19 100780/
PLOG/ 1.0000 6.14E+68 -16.15 105890/
PLOG/ 10.0000 9.70E+66 -15.301 109000/

PLOG/ 100.0000 1.45E+62 -13.64 110210/
 DUP
 IC4H8<=>CCYCCC 1.000E+011 0.000 0.0
 PLOG/ 0.0100 4.84E+41 -9.62 79528/
 PLOG/ 0.1000 8.07E+44 -10.21 82671/
 PLOG/ 1.0000 1.15E+47 -10.56 85502/
 PLOG/ 10.0000 1.33E+39 -7.98 83303/
 PLOG/ 100.0000 4.97E+31 -5.6 80987/
 DUP

CCYCCC<=>IC4H7+H 1.000E+011 0.000
 0.0
 PLOG/ 0.0100 2.33E+63 -14.55 103320/
 PLOG/ 0.1000 7.03E+63 -14.37 107160/
 PLOG/ 1.0000 5.07E+64 -14.29 112340/
 PLOG/ 10.0000 4.92E+61 -13.15 114870/
 PLOG/ 100.0000 4.82E+57 -11.73 118250/
 DUP

CCYCCC<=>IC4H7+H 1.000E+011 0.000
 0.0
 PLOG/ 0.0100 1.12E+40 -8.37 85836/
 PLOG/ 0.1000 1.06E+41 -8.33 88499/
 PLOG/ 1.0000 8.23E+43 -8.88 92907/
 PLOG/ 10.0000 1.27E+39 -7.33 93401/
 PLOG/ 100.0000 1.45E+28 -4.02 90995/
 DUP

CCYCCC<=>C3H5-T+CH3 1.000E+011 0.000
 0.0
 PLOG/ 0.0100 8.31E+64 -15.14 111300/
 PLOG/ 0.1000 8.29E+64 -14.72 113700/
 PLOG/ 1.0000 1.00E+70 -15.72 121940/
 PLOG/ 10.0000 1.66E+67 -14.59 124380/
 PLOG/ 100.0000 7.87E+62 -13.05 126800/
 DUP

CCYCCC<=>C3H5-T+CH3 1.000E+011 0.000
 0.0
 PLOG/ 0.0100 1.51E+49 -11.04 99748/
 PLOG/ 0.1000 1.05E+45 -9.46 99275/
 PLOG/ 1.0000 3.39E+50 -10.63 104220/
 PLOG/ 10.0000 1.76E+47 -9.43 104930/
 PLOG/ 100.0000 1.88E+39 -6.93 103980/
 DUP

!CZ 27/01/2014

!!REF:LASKIN ET AL. IJCK 32 589-614 2000

!C3H5-T+CH3 (+M) <=>IC4H8 (+M) 2.500E+013 0.000

0.0

!LOW/ 4.270E+058 -11.940

9769.8/

!TROE/ 1.750E-001 1.341E+003 6.000E+004 1.014E+004/

!IC4H7+H (+M) <=>IC4H8 (+M) 1.000E+014 0.000

0.0

!LOW/ 6.650E+059 -12.000

5967.8/

!TROE/ 2.000E-002 1.097E+003 1.097E+003 6.860E+003/

!H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/

IC4H8<=>IC4H7-I1+H 7.710E+069 -16.090
140000.0

!REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H<=>IC4H9 1.000E+000 1.000
0.0

PLOG/	0.0013	7.990E+081	-23.161	22239.0/
PLOG/	0.0400	4.240E+068	-18.427	19665.0/
PLOG/	1.0000	1.040E+049	-11.500	15359.0/
PLOG/	10.0000	6.200E+041	-8.892	14637.0/
!PLOG/	100.0000	-6.450E+031	-5.851	8177.8/

DUP

IC4H8+H<=>IC4H9 1.000E+000 1.000
0.0

PLOG/	0.0013	1.850E+026	-5.830	3865.8/
PLOG/	0.0400	2.820E+030	-6.490	5470.8/
PLOG/	1.0000	3.780E+028	-5.570	5625.1/
PLOG/	10.0000	1.460E+025	-4.280	5247.8/

!REF: REFIT TO ONE PARAMETER TO AVOID PROBLEMS WITH NEGATIVE K

PLOG/	100.0000	4.220E+027	-4.390	9345.8/
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DUP

IC4H8+H<=>C3H6+CH3 1.000E+000 1.000
1.0

PLOG/	0.0013	1.540E+009	1.350	2542.0/
PLOG/	0.0400	7.880E+010	0.870	3599.6/
PLOG/	1.0000	2.670E+012	0.470	5431.1/
PLOG/	10.0000	9.250E+022	-2.600	12898.0/
PLOG/	100.0000	1.320E+023	-2.420	16500.0/

DUP

IC4H8+H<=>C3H6+CH3 1.000E+000 1.000
1.0

PLOG/	10.0000	1.240E+005	2.520	3679.1/
PLOG/	100.0000	2.510E+003	2.910	3980.9/

DUP

IC4H8+H<=>TC4H9 1.000E+000 1.000
1.0

PLOG/	0.0013	1.350E+044	-10.680	8196.4/
PLOG/	0.0400	2.110E+057	-14.230	15147.0/
PLOG/	1.0000	3.260E+061	-14.940	20161.0/
PLOG/	10.0000	5.300E+056	-13.120	20667.0/
PLOG/	100.0000	1.110E+050	-10.800	20202.0/

DUP

IC4H8+H<=>TC4H9 1.000E+000 1.000
1.0

PLOG/	0.0013	2.170E+130	-32.580	136140.0/
PLOG/	0.0400	2.250E+029	-5.840	4241.9/
PLOG/	1.0000	1.060E+030	-5.630	5613.4/
PLOG/	10.0000	6.110E+026	-4.440	5182.3/
PLOG/	100.0000	2.730E+023	-3.260	4597.0/

DUP

!C3H6+CH3<=>IC4H9 1.000E+000 1.000
1.0

!PLOG/	0.0013	8.670E+048	-12.540	18206.0/
!PLOG/	0.0400	1.060E+049	-12.040	20001.0/
!PLOG/	1.0000	7.670E+047	-11.170	22366.0/

!PLOG/	10.0000	1.810E+045	-10.030	23769.0/	
!PLOG/	100.0000	2.040E+040	-8.250	24214.0/	
!DUP					
!C3H6+CH3<=>IC4H9				1.000E+000	1.000
1.0					
!PLOG/	0.0013	1.120E+043	-11.300	13080.0/	
!PLOG/	0.0400	7.280E+039	-9.880	13164.0/	
!PLOG/	1.0000	2.600E+033	-7.460	12416.0/	
!PLOG/	10.0000	3.850E+027	-5.380	11455.0/	
!PLOG/	100.0000	1.660E+021	-3.170	10241.0/	
!DUP					

! FROM K. ZHANG ESTIMATED
 IC4H9<=>C3H6+CH3 1.0 1.0 1.0
 PLOG / 1.000E-001 3.150E+041 -9.50 33486. / !FIT FROM: 500-2000 K
 ERROR IN FIT: 34%
 PLOG / 1.000E+000 6.750E+044 -10.07 37209. / !FIT FROM: 500-2000 K
 ERROR IN FIT: 29%
 PLOG / 1.000E+001 7.790E+044 -9.70 39751. / !FIT FROM: 500-2000 K
 ERROR IN FIT: 19%
 PLOG / 1.000E+002 3.610E+039 -7.78 39583. / !FIT FROM: 500-2000 K
 ERROR IN FIT: 10%

IC4H8+H<=>IC4H7+H2	7.29E+05	2.455
4361.2		
IC4H8+H<=>IC4H7-I1+H2	8.621E+02	3.25
12166.98		

!REF: F. GOLDSMITH JPCA, 2012		
IC4H9+O2<=>IC4H9O2	6.6946E+13	-0.3 -
187.2		
TC4H9+O2<=>TC4H9O2	6.6946E+13	-0.3 -
187.2		

!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
IC4H9O2<=>IC4H8O2H-I	9.82E+07	1.3
21500		
IC4H9O2<=>IC4H8O2H-T	2.31E+09	0.8
27100		
TC4H9O2<=>TC4H8O2H-I	4.521E+009	1.2
33500.0		

!REF:GOLDSMITH, JPCA, 2012		
IC4H8O2H-I+O2<=>IC4H8OOH-IO2	9.35316E+11	0.1 -
1010.88		
IC4H8O2H-T+O2<=>IC4H8OOH-TO2	5.04482E+12	-0.1 -
655.2		
TC4H8O2H-I+O2<=>TC4H8OOH-IO2	22844293817	0.5 -
786.24		

!REF:GREEN 2003		
IC4H8O2H-I<=>CC4H8O+OH	4.470E+011	0.000
21900.0		
!REF:		
IC4H8O2H-I=>OH+CH2O+C3H6	8.451E+015	-0.680
29170.0		

TC4H8OOH-IO2<=>TIC4H7Q2-I 21500.0	9.820E+007	1.300
TIC4H7Q2-I<=>IC4H7OOH+HO2 15200.0	1.600E+012	0.230

! REF:

IC4H8OOH-IO2<=>IC4KETII+OH 21400.0	5.000E+010	0.000
IC4H8OOH-IO2<=>IIC4H7Q2-I 24400.0	3.750E+010	0.000
IC4H8OOH-IO2<=>IIC4H7Q2-T 29200.0	1.000E+011	0.000

! CURRAN ESTIMATED

IC4KETII=>CH2O+C2H5CO+OH 42000.0	1.500E+016	0.000
AC3H5OOH+CH2O2H<=>IIC4H7Q2-I 10600.0	8.500E+010	0.000
IC4H7OOH+HO2<=>IIC4H7Q2-T 7800.0	1.000E+011	0.000

! REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY

! IC4H8+OH<=>IC4H7+H2O 2.67841 -827.103	43950.16898	
! IC4H8+OH<=>IC4H7-I1+H2O 1114.19989	5465.0474	2.81477

! MULTIPLY BY 1.2 FROM THE ABOVE

IC4H8+OH<=>IC4H7+H2O -827.17	52740.24	2.7
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! DIVIDED BY 2 FROM THE ABOVE

! IC4H8+OH<=>IC4H7+H2O 2.67841 -827.103	21975.08449	
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! MULTIPLY BY 2 FROM THE ABOVE

IC4H8+OH<=>IC4H7-I1+H2O 1114.19989	10930.0948	2.81477
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! ANALOGY TO C3H6+OH

IC4H8+OH<=>IC4H7OH+H 10580.0	2.290E+013	0.070
PLOG/ 0.0013 2.670E+013 0.050 10611.0/		
PLOG/ 0.0100 2.750E+013 0.050 10623.0/		
PLOG/ 0.0130 2.870E+013 0.040 10634.0/		
PLOG/ 0.0250 1.590E+014 -0.160 11125.0/		
PLOG/ 0.1000 3.100E+014 -0.220 11407.0/		
PLOG/ 0.1315 3.780E+014 -0.240 11458.0/		
PLOG/ 1.0000 9.150E+007 1.420 10087.0/		
PLOG/ 10.0000 3.660E+005 2.140 10410.0/		
PLOG/ 100.0000 8.190E+002 2.840 10481.0/		
IC4H8+OH<=>SC3H5OH+CH3 1233.0	1.290E+006	1.650
PLOG/ 0.0013 5.16E+05 1.650 1233.0/		
PLOG/ 0.0100 7.28E+03 2.100 1162.0/		
PLOG/ 0.0130 8.16E+02 2.480 1128.0/		

PLOG/	0.0250	1.15E+02	2.800	1152.0/		
PLOG/	0.1000	5.60E+00	3.210	1208.0/		
PLOG/	0.1315	3.08E+00	3.290	1216.0/		
PLOG/	1.0000	4.52E+03	2.500	3238.0/		
PLOG/	10.0000	9.64E+18	-1.740	13107.0/		
PLOG/	100.0000	1.32E-01	3.700	3665.0/		
IC4H8+OH<=>IC3H5OH+CH3					1.290E+006	1.650
1233.0						
PLOG/	0.0013	2.06E+06	1.650	1233.0/		
PLOG/	0.0100	2.91E+04	2.100	1162.0/		
PLOG/	0.0130	3.26E+03	2.480	1128.0/		
PLOG/	0.0250	4.61E+02	2.800	1152.0/		
PLOG/	0.1000	2.24E+01	3.210	1208.0/		
PLOG/	0.1315	1.23E+01	3.290	1216.0/		
PLOG/	1.0000	1.81E+04	2.500	3238.0/		
PLOG/	10.0000	3.86E+19	-1.740	13107.0/		
PLOG/	100.0000	5.28E-01	3.700	3665.0/		
IC4H8+OH<=>SC4H7OH-I+H					2.870E+000	2.920
625.0						
PLOG/	0.0013	2.870E+000	2.920	625.0/		
PLOG/	0.0100	4.840E-001	2.980	704.0/		
PLOG/	0.0130	3.130E-001	3.040	721.0/		
PLOG/	0.0250	9.330E-003	3.620	677.0/		
PLOG/	0.1000	4.640E-005	4.480	687.0/		
PLOG/	0.1315	2.710E-005	4.560	707.0/		
PLOG/	1.0000	7.650E-007	5.050	874.0/		
PLOG/	10.0000	2.640E+015	-0.800	12728.0/		
PLOG/	100.0000	4.870E-004	4.320	4020.0/		
IC4H8+OH<=>CH3COCH3+CH3					6.930E+005	1.490
-536.0						
PLOG/	0.0013	6.930E+005	1.490	-536.0/		
PLOG/	0.0100	5.940E+003	2.010	-560.0/		
PLOG/	0.0130	1.100E+003	2.220	-680.0/		
PLOG/	0.0250	1.070E+002	2.500	-759.0/		
PLOG/	0.1000	7.830E-001	3.100	-919.0/		
PLOG/	0.1315	3.070E-001	3.220	-946.0/		
PLOG/	1.0000	3.160E-004	4.050	-1144.0/		
PLOG/	10.0000	7.590E-006	4.490	-680.0/		
PLOG/	100.0000	5.450E-005	4.220	1141.0/		
!IC4H8+OH<=>IC4H8OH-IT					5.100E+054	-20.700
32402.0						
!PLOG/	0.0013	3.07E+78	-20.7	32402/		
!PLOG/	0.0100	3.65E+77	-20	33874/		
!PLOG/	0.0130	1.42E+76	-19.58	32874/		
!PLOG/	0.0250	4.90E+73	-18.79	31361/		
!PLOG/	0.1000	1.38E+68	-17.01	27909/		
!PLOG/	0.1315	9.64E+66	-16.64	27162/		
!PLOG/	1.0000	2.60E+59	-14.17	23079/		
!PLOG/	10.0000	1.01E+54	-12.23	22976/		
!PLOG/	100.0000	1.91E+48	-10.23	23772/		
!DUP						
!IC4H8+OH<=>IC4H8OH-IT					1.420E+036	-15.840
11594.0						
!PLOG/	0.0013	8.55E+59	-15.84	11594/		
!PLOG/	0.0100	9.70E+59	-15.51	12898/		
!PLOG/	0.0130	3.72E+59	-15.34	12913/		
!PLOG/	0.0250	3.53E+58	-14.93	12936/		
!PLOG/	0.1000	1.80E+56	-14.04	12945/		

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!PLOG/      0.1315      5.31E+55      -13.85      12887/
!PLOG/      1.0000      2.07E+50      -12.04      11493/
!PLOG/     10.0000      8.55E+41      -9.35 8921/
!PLOG/    100.0000      3.06E+32      -6.31 6088/
!DUP
!IC4H8+OH<=>IC4H8OH-TI                                5.100E+054      -20.700
32402.0
!PLOG/      0.0013      3.07E+78      -20.7 32402/
!PLOG/      0.0100      3.65E+77      -20          33874/
!PLOG/      0.0130      1.42E+76      -19.58      32874/
!PLOG/      0.0250      4.90E+73      -18.79      31361/
!PLOG/      0.1000      1.38E+68      -17.01      27909/
!PLOG/      0.1315      9.64E+66      -16.64      27162/
!PLOG/      1.0000      2.60E+59      -14.17      23079/
!PLOG/     10.0000      1.01E+54      -12.23      22976/
!PLOG/    100.0000      1.91E+48      -10.23      23772/
!DUP
!IC4H8+OH<=>IC4H8OH-TI                                1.420E+036      -15.840
11594.0
!PLOG/      0.0013      8.55E+59      -15.84      11594/
!PLOG/      0.0100      9.70E+59      -15.51      12898/
!PLOG/      0.0130      3.72E+59      -15.34      12913/
!PLOG/      0.0250      3.53E+58      -14.93      12936/
!PLOG/      0.1000      1.80E+56      -14.04      12945/
!PLOG/      0.1315      5.31E+55      -13.85      12887/
!PLOG/      1.0000      2.07E+50      -12.04      11493/
!PLOG/     10.0000      8.55E+41      -9.35 8921/
!PLOG/    100.0000      3.06E+32      -6.31 6088/
!DUP

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! INCREASE THE ABOVE BY A FACTOR OF 2 FOR TEST

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IC4H8+OH<=>IC4H8OH-IT                                5.100E+054      -20.700
32402.0
PLOG/      0.0013      6.14E+78      -20.7 32402/
PLOG/      0.0100      7.30E+77      -20          33874/
PLOG/      0.0130      2.84E+76      -19.58      32874/
PLOG/      0.0250      9.80E+73      -18.79      31361/
PLOG/      0.1000      2.76E+68      -17.01      27909/
PLOG/      0.1315      1.93E+67      -16.64      27162/
PLOG/      1.0000      5.20E+59      -14.17      23079/
PLOG/     10.0000      2.02E+54      -12.23      22976/
PLOG/    100.0000      3.82E+48      -10.23      23772/
DUP
IC4H8+OH<=>IC4H8OH-IT                                1.420E+036      -15.840
11594.0
PLOG/      0.0013      1.71E+60      -15.84      11594/
PLOG/      0.0100      1.94E+60      -15.51      12898/
PLOG/      0.0130      7.44E+59      -15.34      12913/
PLOG/      0.0250      7.06E+58      -14.93      12936/
PLOG/      0.1000      3.60E+56      -14.04      12945/
PLOG/      0.1315      1.06E+56      -13.85      12887/
PLOG/      1.0000      4.14E+50      -12.04      11493/
PLOG/     10.0000      1.71E+42      -9.35 8921/
PLOG/    100.0000      6.12E+32      -6.31 6088/
DUP

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! DECREASE THE ABOVE BY A FACTOR OF 2 FROM THE CH3
IC4H8+OH<=>IC4H8OH-TI 5.100E+054 -20.700
32402.0

PLOG/	0.0013	1.54E+78	-20.7	32402/
PLOG/	0.0100	1.83E+77	-20	33874/
PLOG/	0.0130	7.10E+75	-19.58	32874/
PLOG/	0.0250	2.45E+73	-18.79	31361/
PLOG/	0.1000	6.90E+67	-17.01	27909/
PLOG/	0.1315	4.82E+66	-16.64	27162/
PLOG/	1.0000	1.30E+59	-14.17	23079/
PLOG/	10.0000	5.05E+53	-12.23	22976/
PLOG/	100.0000	9.55E+47	-10.23	23772/

DUP

IC4H8+OH<=>IC4H8OH-TI 1.420E+036 -15.840
11594.0

PLOG/	0.0013	4.28E+59	-15.84	11594/
PLOG/	0.0100	4.85E+59	-15.51	12898/
PLOG/	0.0130	1.86E+59	-15.34	12913/
PLOG/	0.0250	1.77E+58	-14.93	12936/
PLOG/	0.1000	9.00E+55	-14.04	12945/
PLOG/	0.1315	2.66E+55	-13.85	12887/
PLOG/	1.0000	1.04E+50	-12.04	11493/
PLOG/	10.0000	4.28E+41	-9.35	8921/
PLOG/	100.0000	1.53E+32	-6.31	6088/

DUP

! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
IC4H8OH-IT+O2<=>TQJC4H8OH 1.420E+036 -15.840 11594.0

PLOG/	0.001	1.05E+114	-33.81	24741/
PLOG/	0.01	2.13E+114	-33.44	26448/
PLOG/	0.1	1.62E+110	-31.75	26612/
PLOG/	1	6.00E+101	-28.79	25197/
PLOG/	10	5.36E+89	-24.76	22402/
PLOG/	40	1.55E+81	-21.95	20197/
PLOG/	100	1.51E+75	-20	18578/
PLOG/	200	3.16E+70	-18.48	17287/

IC4H8OH-IT+O2<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0

PLOG/	0.001	1.21E+26	-5.09	5755/
PLOG/	0.01	1.41E+31	-6.55	8781/
PLOG/	0.1	5.08E+34	-7.53	11702/
PLOG/	1	1.67E+34	-7.27	13418/
PLOG/	10	2.82E+28	-5.41	13318/
PLOG/	40	2.50E+22	-3.52	12314/
PLOG/	100	2.82E+17	-1.99	11286/
PLOG/	200	1.93E+13	-0.71	10340/

DUP

IC4H8OH-IT+O2<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0

PLOG/	0.001	2.45E+21	-4.19	6837/
PLOG/	0.01	1.40E+30	-6.75	11554/
PLOG/	0.1	9.11E+39	-9.56	17834/
PLOG/	1	5.16E+42	-10.17	22412/
PLOG/	10	6.07E+32	-6.94	22738/
PLOG/	40	3.88E+20	-3.14	20677/
PLOG/	100	3.32E+10	-0.03	18552/
PLOG/	200	1.22E+02	2.57	16623/

DUP

IC4H8OH-IT+O2<=>SC4H7OH-I+HO2		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.26E+25	-4.69	5755/
PLOG/	0.01	1.44E+30	-6.15	8785/
PLOG/	0.1	4.78E+33	-7.11	11695/
PLOG/	1	1.40E+33	-6.84	13395/
PLOG/	10	2.12E+27	-4.96	13277/
PLOG/	40	1.78E+21	-3.07	12265/
PLOG/	100	1.97E+16	-1.53	11234/
PLOG/	200	1.32E+12	-0.25	10285/
DUP				
IC4H8OH-IT+O2<=>SC4H7OH-I+HO2		1.420E+036	-15.840	11594.0
PLOG/	0.001	3.22E+23	-4.69	5341/
PLOG/	0.01	4.80E+28	-6.18	8461/
PLOG/	0.1	1.71E+32	-7.16	11410/
PLOG/	1	1.53E+32	-7.02	13378/
PLOG/	10	5.55E+29	-6.14	15100/
PLOG/	40	1.72E+26	-4.97	15849/
PLOG/	100	4.46E+21	-3.51	15644/
PLOG/	200	5.06E+16	-1.96	14979/
DUP				
IC4H8OH-IT+O2<=>TQC4H8OI		1.420E+036	-15.840	11594.0
PLOG/	0.001	6.36+104	-33.74	22390/
PLOG/	0.01	7.96+103	-33.01	22966/
PLOG/	0.1	6.99E+96	-30.48	20584/
PLOG/	1	1.04E+88	-27.47	16629/
PLOG/	10	3.13E+96	-29.62	20346/
PLOG/	40	2.79+105	-32.04	24971/
PLOG/	100	4.64+109	-33.12	27657/
PLOG/	200	2.06+111	-33.48	29197/
IC4H8OH-IT+O2<=>CH3COCH3+CH2O+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	3.03E+37	-8.35	6940/
PLOG/	0.01	1.07E+42	-9.64	9965/
PLOG/	0.1	9.22E+43	-10.12	12427/
PLOG/	1	1.14E+42	-9.42	13806/
PLOG/	10	1.80E+38	-8.13	15131/
PLOG/	40	1.61E+34	-6.8	15691/
PLOG/	100	7.00E+29	-5.41	15552/
PLOG/	200	3.74E+25	-4.06	15118/
IC4H8OH-IT+O2<=>QC4H7OHP		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.18+118	-37.6	26229 /
PLOG/	0.01	1.91+131	-40.73	34079/
PLOG/	0.1	5.81+138	-42.17	40750/
PLOG/	1	5.05+134	-40.19	43580/
PLOG/	10	2.07+117	-34.26	41516/
PLOG/	40	1.71+101	-29.04	38094/
PLOG/	100	1.25E+89	-25.15	35203/
PLOG/	200	2.98E+79	-22.09	32802/
IC4H8OH-IT+O2<=>CCY(CCO)COH+OH		1.420E+036	-15.840	11594.0
PLOG/	0.001	2.11E+18	-2.87	6870/
PLOG/	0.01	3.02E+27	-5.54	11842/
PLOG/	0.1	1.36E+37	-8.29	18165/
PLOG/	1	1.21E+39	-8.66	22517/
PLOG/	10	1.53E+28	-5.13	22530/
PLOG/	40	2.72E+15	-1.16	20283/
PLOG/	100	1.06E+05	2.06	18044/
PLOG/	200	2.30E-04	4.73	16037/
IC4H8OH-IT+O2<=>TQC4H7OHI		1.420E+036	-15.840	11594.0
PLOG/	0.001	1.76E+53	-19.87	9019/

PLOG/	0.01	4.68E+67	-23.92	11892/		
PLOG/	0.1	2.07E+91	-30.58	17347/		
PLOG/	1	2.84+100	-32.4	20041/		
PLOG/	10	1.16+115	-35.81	27656/		
PLOG/	40	4.87+123	-37.83	33314/		
PLOG/	100	7.95+124	-37.82	35683/		
PLOG/	200	4.58+122	-36.86	36374/		
IC4H8OH-IT+O2<=>C2CY (COC) OH+OH		1.420E+036			-15.840	11594.0
PLOG/	0.001	1.42E+32	-6.95	6210/		
PLOG/	0.01	5.19E+36	-8.24	9233/		
PLOG/	0.1	5.77E+38	-8.76	11715/		
PLOG/	1	2.86E+36	-7.95	12823/		
PLOG/	10	1.37E+32	-6.51	13646/		
PLOG/	40	2.15E+29	-5.56	14541/		
PLOG/	100	1.20E+26	-4.51	14778/		
PLOG/	200	3.31E+22	-3.37	14606/		
TQJC4H8OH<=>IC4H7OH+HO2		1.420E+036			-15.840	11594.0
PLOG/	0.001	9.73E+65	-18.5	42975/		
PLOG/	0.01	1.04E+64	-17.25	44419/		
PLOG/	0.1	7.90E+59	-15.59	44504/		
PLOG/	1	9.35E+53	-13.49	43566/		
PLOG/	10	4.13E+44	-10.39	41279/		
PLOG/	40	6.57E+38	-8.49	39745/		
PLOG/	100	8.32E+34	-7.23	38675/		
PLOG/	200	9.46E+31	-6.28	37849/		
DUP						
TQJC4H8OH<=>IC4H7OH+HO2		1.420E+036			-15.840	11594.0
PLOG/	0.001	5.27E+64	-18	42872/		
PLOG/	0.01	4.82E+62	-16.74	44284/		
PLOG/	0.1	3.42E+58	-15.07	44348/		
PLOG/	1	4.05E+52	-12.97	43402/		
PLOG/	10	1.93E+43	-9.88	41120/		
PLOG/	40	3.28E+37	-7.99	39593/		
PLOG/	100	4.35E+33	-6.74	38527/		
PLOG/	200	5.13E+30	-5.79	37706/		
DUP						
TQJC4H8OH<=>TQC4H8OI		1.420E+036			-15.840	11594.0
PLOG/	0.001	3.78E+50	-12.91	31539/		
PLOG/	0.01	1.42E+45	-10.94	30864/		
PLOG/	0.1	1.50E+40	-9.21	29932/		
PLOG/	1	3.12E+35	-7.64	28864/		
PLOG/	10	2.73E+29	-5.67	27243/		
PLOG/	40	8.88E+25	-4.54	26272/		
PLOG/	100	4.60E+23	-3.8	25622/		
PLOG/	200	9.08E+21	-3.25	25131/		
TQJC4H8OH<=>QC4H7OHP		1.420E+036			-15.840	11594.0
PLOG/	0.001	9.16E+62	-18.02	45297/		
PLOG/	0.01	2.56E+62	-17.1	47393/		
PLOG/	0.1	1.25E+59	-15.61	47984/		
PLOG/	1	1.97E+53	-13.49	47281/		
PLOG/	10	1.91E+43	-10.15	44926/		
PLOG/	40	7.68E+36	-8.05	43267/		
PLOG/	100	3.49E+32	-6.64	42089/		
PLOG/	200	1.77E+29	-5.57	41173/		
TQJC4H8OH<=>TQC4H7OHI		1.420E+036			-15.840	11594.0
PLOG/	0.001	9.57E+58	-15.99	38293/		
PLOG/	0.01	7.27E+54	-14.25	38593/		
PLOG/	0.1	8.30E+49	-12.44	38031/		

PLOG/	1	1.90E+44	-10.51	36905/		
PLOG/	10	2.18E+36	-7.9	34865/		
PLOG/	40	4.10E+31	-6.36	33581/		
PLOG/	100	3.00E+28	-5.35	32704/		
PLOG/	200	1.34E+26	-4.59	32035/		
TQC4H8OI<=>CH3COCH3+CH2O+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	8.09E+38	-9.91	19096/		
PLOG/	0.01	9.09E+39	-9.93	19135/		
PLOG/	0.1	1.89E+41	-10.02	19407/		
PLOG/	1	7.47E+23	-4.1	14658/		
PLOG/	10	2.95E+33	-6.75	18685/		
PLOG/	40	4.24E+36	-7.56	20307/		
PLOG/	100	7.83E+36	-7.54	20747/		
PLOG/	200	7.63E+35	-7.17	20641/		
QC4H7OHP<=>IC4H7OH+HO2		1.420E+036	-15.840		11594.0	
PLOG/	0.001	3.29E+57	-15.64	28576/		
PLOG/	0.01	9.65E+58	-15.75	29927/		
PLOG/	0.1	2.19E+50	-12.66	28547/		
PLOG/	1	1.67E+49	-12.05	29204/		
PLOG/	10	7.08E+40	-9.26	27188/		
PLOG/	40	1.32E+30	-5.82	24071/		
PLOG/	100	1.15E+30	-5.8	24053/		
PLOG/	200	1.12E+30	-5.8	24050/		
QC4H7OHP<=>CCY (CCO) COH+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	1.11E+51	-12.97	28497/		
PLOG/	0.01	5.58E+51	-12.87	29529/		
PLOG/	0.1	3.03E+44	-10.28	28326/		
PLOG/	1	1.42E+44	-9.98	28986/		
PLOG/	10	9.69E+37	-7.93	27491/		
PLOG/	40	5.90E+29	-5.3	25095/		
PLOG/	100	5.27E+29	-5.29	25081/		
PLOG/	200	5.15E+29	-5.28	25078/		
TQC4H7OHI<=>C2CY (COC) OH+OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	1.10E+31	-7.21	14640/		
PLOG/	0.01	1.37E+32	-7.24	14716/		
PLOG/	0.1	3.34E+33	-7.35	15127/		
PLOG/	1	1.86E+23	-3.68	12864/		
PLOG/	10	9.88E+31	-6.23	16040/		
PLOG/	40	1.25E+34	-6.78	17056/		
PLOG/	100	7.73E+33	-6.67	17176/		
PLOG/	200	2.13E+33	-6.45	17170/		
TQC4H7OHI<=>SC4H7OH-I+HO2		1.420E+036	-15.840		11594.0	
PLOG/	0.001	6.01E+27	-7.27	14658/		
PLOG/	0.01	7.78E+28	-7.3	14733/		
PLOG/	0.1	3.27E+30	-7.48	15191/		
PLOG/	1	2.81E+17	-2.82	12336/		
PLOG/	10	1.92E+26	-5.22	16146/		
PLOG/	40	7.61E+27	-5.49	17483/		
PLOG/	100	1.91E+26	-4.86	17429/		
PLOG/	200	2.94E+24	-4.18	17285/		
IC4H8OH-TI+O2<=>IQJC4H8OH		1.420E+036	-15.840		11594.0	
PLOG/	0.001	3.34+111	-32.67	25143/		
PLOG/	0.01	4.84+107	-31.05	25460/		
PLOG/	0.1	2.41+100	-28.42	24474/		
PLOG/	1	4.55E+89	-24.78	22176/		
PLOG/	10	1.14E+76	-20.31	18721/		
PLOG/	40	9.25E+66	-17.35	16238/		

PLOG/	100	6.20E+60	-15.36	14499/		
PLOG/	200	1.30E+56	-13.86	13159/		
IC4H8OH-TI+O2<=>IC3H6OHCHO+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.59E+15	-1.63	8947/		
PLOG/	0.01	5.07E+20	-3.24	11938/		
PLOG/	0.1	5.00E+25	-4.66	15251/		
PLOG/	1	3.18E+26	-4.79	17388/		
PLOG/	10	6.00E+20	-2.95	17297/		
PLOG/	40	1.70E+14	-0.91	16099/		
PLOG/	100	7.91E+08	0.73	14913/		
PLOG/	200	3.03E+04	2.08	13854/		
IC4H8OH-TI+O2<=>IQC4H8OT		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.12+102	-32.4	23496/		
PLOG/	0.01	4.23E+95	-30.04	22067/		
PLOG/	0.1	3.45E+83	-26.08	17114/		
PLOG/	1	8.16E+82	-25.61	16198/		
PLOG/	10	1.04E+97	-29.54	22648/		
PLOG/	40	7.25+103	-31.42	26487/		
PLOG/	100	2.48+106	-32.06	28397/		
PLOG/	200	1.39+107	-32.2	29446/		
IC4H8OH-TI+O2<=>CH3COCH3+CH2O+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	4.39E+48	-11.88	11603/		
PLOG/	0.01	9.82E+50	-12.49	14143/		
PLOG/	0.1	3.43E+49	-11.94	15561/		
PLOG/	1	2.43E+45	-10.56	16415/		
PLOG/	10	4.98E+39	-8.68	17473/		
PLOG/	40	7.99E+33	-6.83	17502/		
PLOG/	100	1.02E+29	-5.28	17165/		
PLOG/	200	7.18E+24	-3.99	16747/		
IC4H8OH-TI+O2<=>CH3+CH3COCOOH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	2.91E+40	-9.23	10830/		
PLOG/	0.01	9.66E+43	-10.2	13698/		
PLOG/	0.1	1.34E+44	-10.13	15661/		
PLOG/	1	2.57E+41	-9.18	17047/		
PLOG/	10	1.82E+36	-7.46	18330/		
PLOG/	40	8.82E+29	-5.44	18205/		
PLOG/	100	1.74E+24	-3.65	17600/		
PLOG/	200	2.16E+19	-2.12	16925/		
IC4H8OH-TI+O2<=>IQC4H7OHT		1.420E+036	-15.840	11594.0		
PLOG/	0.001	1.03+115	-35.13	25407/		
PLOG/	0.01	1.10+129	-38.89	32891/		
PLOG/	0.1	5.15+135	-40.38	38573/		
PLOG/	1	7.27+129	-38.13	39933/		
PLOG/	10	4.50+112	-32.49	37045/		
PLOG/	40	7.72E+97	-27.79	33612/		
PLOG/	100	5.17E+86	-24.26	30799/		
PLOG/	200	4.70E+77	-21.41	28440/		
IC4H8OH-TI+O2<=>IC3H5OH+CH2O+OH		1.420E+036	-15.840	11594.0		
PLOG/	0.001	5.10E+24	-4.31	13009/		
PLOG/	0.01	6.91E+33	-6.97	17935/		
PLOG/	0.1	1.74E+41	-9.03	23613/		
PLOG/	1	2.26E+36	-7.32	25633/		

PLOG/ 10 3.15E+17 -1.4 22782/
PLOG/ 40 9.35E+00 3.71 19114/
PLOG/ 100 5.59E-12 7.46 16156/
PLOG/ 200 1.27E-21 10.41 13733/

IC4H8OH-TI+O2<=>CCY(CCOC)OH+OH 1.420E+036 -15.840 11594.0

PLOG/ 0.001 3.06E+33 -7.24 11476/
PLOG/ 0.01 6.56E+42 -9.92 17197/
PLOG/ 0.1 8.24E+46 -10.95 22090/
PLOG/ 1 4.48E+38 -8.22 23019/
PLOG/ 10 1.01E+18 -1.77 19496/
PLOG/ 40 1.16E+01 3.44 15637/
PLOG/ 100 4.85E-12 7.23 12599/
PLOG/ 200 8.64E-22 10.21 10126/

!

IQJC4H8OH<=>IC3H6OHCHO+OH 1.420E+036 -15.840 11594.0

PLOG/ 0.001 3.58E+71 -20.62 52656/
PLOG/ 0.01 9.67E+71 -20.08 54935/
PLOG/ 0.1 3.39E+67 -18.18 55330/
PLOG/ 1 7.26E+58 -15.09 54016/
PLOG/ 10 4.57E+46 -11.01 51172/
PLOG/ 40 4.31E+38 -8.38 49054/
PLOG/ 100 2.12E+33 -6.66 47587/
PLOG/ 200 2.72E+29 -5.41 46486/

!

IQJC4H8OH<=>IQC4H8OT 1.420E+036 -15.840 11594.0

PLOG/ 0.001 1.04E+45 -11.2 31755/
PLOG/ 0.01 2.90E+40 -9.62 30945/
PLOG/ 0.1 4.85E+35 -8.01 29850/
PLOG/ 1 2.62E+30 -6.28 28498/
PLOG/ 10 3.37E+24 -4.37 26873/
PLOG/ 40 9.75E+20 -3.23 25861/
PLOG/ 100 5.61E+18 -2.52 25208/
PLOG/ 200 1.44E+17 -2.01 24740/

IQJC4H8OH<=>IQC4H7OHT 1.420E+036 -15.840 11594.0

PLOG/ 0.001 1.36E+50 -12.93 36743/
PLOG/ 0.01 3.36E+45 -11.27 36143/
PLOG/ 0.1 1.13E+40 -9.41 34990/
PLOG/ 1 5.93E+33 -7.33 33438/
PLOG/ 10 4.24E+26 -5 31502/
PLOG/ 40 1.97E+22 -3.61 30275/
PLOG/ 100 3.43E+19 -2.72 29477/
PLOG/ 200 3.69E+17 -2.09 28900/

!IQC4H8OT<=>CH3COCH3+CH2O+OH 1.420E+036 -15.840 11594.0

!PLOG/ 0.001 9.82E+39-9.95 20737/
!PLOG/ 0.01 1.19E+41-9.97 20814/
!PLOG/ 0.1 2.60E+42-10.07 21229/
!PLOG/ 1 2.63E+32-6.47 19139/
!PLOG/ 10 1.32E+40-8.68 22120/
!PLOG/ 40 4.04E+41-9.03 23000/
!PLOG/ 100 9.07E+40-8.77 23008/
!PLOG/ 200 6.70E+39-8.38 22782/

!IQC4H8OT<=>CH3+CH3COCOCH3 1.420E+036 -15.840 11594.0

!PLOG/ 0.001 2.04E+37-9.27 20741/
!PLOG/ 0.01 2.54E+38-9.29 20821/

!PLOG/ 0.1 7.13E+39-9.42 21267/
!PLOG/ 1 2.95E+28-5.34 18891/
!PLOG/ 10 1.31E+36-7.46 22106/
!PLOG/ 40 2.19E+37-7.68 23084/
!PLOG/ 100 1.39E+36-7.22 23018/
!PLOG/ 200 2.67E+34-6.63 22672/

IQC4H7OHT<=>IC3H5OH+CH2O+OH 1.420E+036 -15.840 11594.0
PLOG/ 0.001 4.25E+16 -3.66 19364/
PLOG/ 0.01 2.98E+33 -8.01 27106/
PLOG/ 0.1 3.46E+38 -8.83 31412/
PLOG/ 1 7.07E+28 -5.46 29633/
PLOG/ 10 2.01E+13 -0.43 25278/
PLOG/ 40 1.43E+13 -0.38 25238/
PLOG/ 100 1.38E+13 -0.38 25234/
PLOG/ 200 1.37E+13 -0.37 25233/

IQC4H7OHT<=>CCY (CCOC) OH+OH 1.420E+036 -15.840 11594.0
PLOG/ 0.001 1.12E+25 -5.59 19349/
PLOG/ 0.01 7.20E+32 -7.6 23093/
PLOG/ 0.1 2.22E+34 -7.65 25130/
PLOG/ 1 2.40E+27 -5.28 23663/
PLOG/ 10 2.24E+17 -2.04 20810/
PLOG/ 40 1.82E+17 -2.01 20786/
PLOG/ 100 1.78E+17 -2.01 20783/
PLOG/ 200 1.77E+17 -2.01 20782/

IQC4H7OHT<=>IC4H7OOH+OH 1.420E+036 -15.840 11594.0
PLOG/ 0.001 6.07E+13 -4.21 22478/
PLOG/ 0.01 9.74E+39 -10.89 33616/
PLOG/ 0.1 2.18E+49 -12.65 40359/
PLOG/ 1 3.32E+37 -8.42 38539/
PLOG/ 10 2.34E+16 -1.56 32712/
PLOG/ 40 1.44E+16 -1.49 32656/
PLOG/ 100 1.38E+16 -1.48 32651/
PLOG/ 200 1.37E+16 -1.48 32649/

!!DIVIDED BY 5

!IC4H8OH-IT+O2<=>C2CY (COC) OH+OH 1.420E+036 -15.840 11594.0
!PLOG/ 0.001 2.84E+31 -6.95 6210/
!PLOG/ 0.01 1.04E+36 -8.24 9233/
!PLOG/ 0.1 1.15E+38 -8.76 11715/
!PLOG/ 1 5.72E+35 -7.95 12823/
!PLOG/ 10 2.74E+31 -6.51 13646/
!PLOG/ 40 4.30E+28 -5.56 14541/
!PLOG/ 100 2.40E+25 -4.51 14778/
!PLOG/ 200 6.62E+21 -3.37 14606/
!

!TQC4H7OHI<=>C2CY (COC) OH+OH 1.420E+036 -15.840 11594.0
!PLOG/ 0.001 2.20E+30-7.21 14640/
!PLOG/ 0.01 2.74E+31-7.24 14716/
!PLOG/ 0.1 6.68E+32-7.35 15127/
!PLOG/ 1 3.72E+22-3.68 12864/
!PLOG/ 10 1.98E+31-6.23 16040/
!PLOG/ 40 2.50E+33-6.78 17056/
!PLOG/ 100 1.55E+33-6.67 17176/
!PLOG/ 200 4.26E+32-6.45 17170/

!

!!MULTIPLY BY 2.0

!TQJC4H8OH<=>TQC4H7OHI	1.420E+036	-15.840	11594.0
!PLOG/ 0.001	1.91E+59-15.99	38293/	
!PLOG/ 0.01	1.45E+55-14.25	38593/	
!PLOG/ 0.1	1.66E+50-12.44	38031/	
!PLOG/ 1	3.80E+44-10.51	36905/	
!PLOG/ 10	4.36E+36-7.9	34865/	
!PLOG/ 40	8.20E+31-6.36	33581/	
!PLOG/ 100	6.00E+28-5.35	32704/	
!PLOG/ 200	2.68E+26-4.59	32035/	

!ANALOGY TO IC4H7OOH DECOMPOSITION

CH3COCOCH2O<=>CH3COCH2O+OH			1.000E+011
0.000 0.0			
PLOG/ 0.0100	1.490E+058	-13.900	54266.9/
PLOG/ 0.1000	1.800E+054	-12.400	54193.8/
PLOG/ 1.0000	3.360E+046	-9.810	52468.5/
PLOG/ 10.0000	2.390E+036	-6.540	49429.0/
PLOG/ 100.0000	1.280E+027	-3.610	46333.1/

!REF: A-FACTOR BY ANALOGY WITH C2H5+CH2O<=>NC3H7O AND EA FROM DHRXN AND IP.

!REF: H. J. CURRAN, INT. J. CHEM. KINET. 38 (4) (2006) 250-275.

!REF: REVERSED REACTION.

CH3COCH2O<=>CH3CO+CH2O	5.872E+20	-2.4218
10535.8		

! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233

C2CY (COC) OH+OH=>IC3H6CO+OH+H2O	2.26E3	2.73	
-4688			
CCY (CCO) COH+OH=>IC3H5CHO+OH+H2O	5.66E2	2.93	-
4039.4			
CCY (CCOC) OH+OH=>CH2O+SC3H4OH+H2O	5.66E2	2.93	-
4039.4			

! J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308

C2CY (COC) OH+HO2=>IC3H6CO+OH+H2O2	8.6	3.46
9732.326		
CCY (CCO) COH+HO2=>IC3H5CHO+OH+H2O2	1.81E-1	3.98
9056.7		
CCY (CCOC) OH+HO2=>CH2O+SC3H4OH+H2O2	1.81E-1	3.98
9056.7		

! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, COMBUST AND FLAME, 2011, 158, 726-731

CCY (CCO) COH+OH=>PC3H4OH-2+CH2O+H2O	1.26E3	2.97	-
2660.6			

! C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, IJCK, 2012, 44, 155-164

CCY (CCO) COH+HO2=>PC3H4OH-2+CH2O+H2O2	1.4E-5	5.26
8267.9		

!REF: J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.

IC3H6OHCHO+OH=>TC3H6OH+CO+H2O	61329.9	2.65	-
4586.4			

IC3H6OHCHO+H=>TC3H6OH+CO+H2	8.66E5	2.3	1426
IC3H6OHCHO+HO2=>TC3H6OH+CO+H2O2	1.01E-4	5.0	3429
IC3H6OHCHO+CH3=>TC3H6OH+CO+CH4	3.94	3.6	4223

TC3H6OH<=>CH3COCH3+H 3.299E+04	8.981E11	0.271	
TC3H6OH<=>IC3H5OH+H 4.090E+04	4.211E10	1.005	
TC3H6OH+O2<=>CH3COCH3+HO2 0.000E+00	2.230E13	0.000	

! C ZHOU ESTIMATED SECOND-O2 ADDITION FROM JOE'S CALCULATION

!TQC4H7OHI+O2<=>TQC4H7OHIO2	3.6E+12	0.0	0.0
!TQC4H7OHIO2<=>TQC4H7OHIQ-I	2.91E+12	-0.226	22300
!TQC4H7OHIQ-I<=>HO2CHO+CH3COCH3+OH	5.36E+12	-0.08	10790
!TQC4H7OHIQ-I<=>IC4KETIT+HO2	2.44E+13	-0.253	32590
!IC4KETIT<=>CH3COCH3+HCO+OH	9.500E+015	0.000	42540.0
!IC4KETIT+OH<=>TC3H6O2HCO+H2O 4586.39996	61329.94775	2.65419	-
!IC4KETIT+HO2<=>TC3H6O2HCO+H2O2 3684.27444	1.1773E-4	4.91966	
!TC3H6O2HCO=>CH3COCH3+CO+OH	4.244E+018	-1.430	4800.0
!TQC4H7OHIO2<=>TQC4H7OHIQ-P	4.33E+9	0.433	26520
!TQC4H7OHIQ-P<=>IC3H5COHQ+HO2	6.12E+13	-0.988	15930
!TQC4H7OHIQ-P<=>CH2CQCOHQ+CH3	5.38E+11	0.070	24800
!TQC4H7OHIQ-P<=>IC3H5Q+HOCHO+OH	5.38E+11	0.070	24800
!TQC4H7OHIQ-P<=>COHQCYC (COC) +OH	1.58E+06	1.613	12600
!TQC4H7OHIQ-P<=>QCYC (CCOC) OH+OH	7.06E+09	0.184	17210
!IC3H5COHQ=>HOCHO+C3H5-T+OH 42879.46	1.59E+20	-1.5	
!CH2CQCOHQ<=>HOCHO+CH2CO+2OH 42879.46	1.59E+20	-1.5	
!CH2CQCOHQ<=>HCO+CH2CO+3OH 42879.46	1.59E+20	-1.5	
!IC3H5Q=>CH2CO+CH3+OH 42879.46	1.59E+20	-1.5	
!COHQCYC (COC) =>HOCHO+CH2O+C2H3+OH 42879.46	1.59E+20	-1.5	
!QCYC (CCOC) OH=>HOCHO+CH2CO+CH3+OH 42879.46	1.59E+20	-1.5	

! C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION

! ANALOGY TO O2 + QOOH_2			
!TQC4H7OHI+O2<=>TQC4H7OHIO2	5.05E+12	-0.1	-695.45
TQC4H7OHIO2<=>TQC4H7OHIQ-I	2.56E+12	-0.13	34360
TQC4H7OHIQ-I<=>HO2CHO+CH3COCH3+OH	5.819E+05	2.40	22790
TQC4H7OHIQ-I<=>IC4KETIT+HO2	1.829E+10	0.790	15100
IC4KETIT<=>CH3COCH3+HCO+OH	9.500E+015	0.000	42540.0
IC4KETIT+OH<=>TC3H6O2HCO+H2O 4586.39996	61329.94775	2.65419	-
IC4KETIT+HO2<=>TC3H6O2HCO+H2O2 3684.27444	1.1773E-4	4.91966	
TC3H6O2HCO=>CH3COCH3+CO+OH	1.278E+020	-1.890	34460.0
TQC4H7OHIO2<=>TQC4H7OHIQ-P 21850	5.69E+08	7.80E-01	
TQC4H7OHIQ-P<=>IC3H5COHQ+HO2 15100	1.83E+10	7.90E-01	

TQC4H7OHIQ-P<=>CH2CQCOHQ+CH3	5.38E+11	0.070	24800
TQC4H7OHIQ-P<=>IC3H5Q+HOCHO+OH	5.38E+11	0.070	24800
TQC4H7OHIQ-P<=>COHQCYC (COC) +OH	2.28E+08	1.29E+00	9890
TQC4H7OHIQ-P<=>QCYC (CCOC) OH+OH	4.58E+15	-1.08E+00	
18440			
IC3H5COHQ=>HOCHO+C3H5-T+OH	1.59E+20	-1.5	
42879.46			
CH2CQCOHQ=>HOCHO+CH2CO+2OH	1.59E+20	-1.5	
42879.46			
CH2CQCOHQ=>HCO+CH2CO+3OH	1.59E+20	-1.5	
42879.46			
IC3H5Q=>CH2CO+CH3+OH	1.59E+20	-1.5	
42879.46			
COHQCYC (COC) =>HOCHO+CH2O+C2H3+OH	1.59E+20	-1.5	
42879.46			
QCYC (CCOC) OH=>HOCHO+CH2CO+CH3+OH	1.59E+20	-1.5	
42879.46			
!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-			
5701			
TQC4H7OHIQ2<=>TQC4H7OHTO2	2.956E+09	0.04	16350
TQC4H7OHTO2<=>HOCOCQ (CH3) 2+OH	1.75E+8	1.7	26000
HOCOCQ (CH3) 2=>CO+CH3COCH3+2OH	1.59E+20	-1.5	
42879.46			
! IQC4H7OHT+O2<=>IQC4H7OHTO2			
IQC4H7OHTO2<=>IQC4H7OHTQ-P	9.35626E+11	0.1	-1072.98
IQC4H7OHTQ-P=>OH+CH2O+CH2COHCH2OOH	2.063E+07	1.0	21070
CH2COHCH2OOH=>OH+CH2O+CH2CO+H	1.20E+10	0.35	15700
42879.46	1.59E+20	-1.5	
IQC4H7OHTQ-P<=>OH+CH2C (CH2OOH) 2	1.0E+11	0.0	0.0
PLOG/ 0.01 2.53E+040 -9.91 32631.4/			
PLOG/ 0.1 2.54E+037 -8.72 32909.5/			
PLOG/ 1 1.12E+031 -6.53 31806.6/			
PLOG/ 10 1.98E+021 -3.34 29137.8/			
PLOG/ 100 1.95E+010 0.154 25612/			
CH2C (CH2OOH) 2=>OH+CH2O+HO2+C3H4-A	1.59E+20	-1.5	
42879.46			
IQC4H7OHTO2<=>IQC4H8OTQ-I	4.13E+07	1.0	21070
IQC4H8OTQ-I=>OH+CH2O+C3KET21	1.20E+10	0.35	15700
C3KET21=>OH+CH2O+CO+CH3	1.59E+20	-1.5	
42879.46			
IQC4H8OTQ-I<=>CH3+CO (CH2OOH) 2	2.740E+13	0.24	29830
CO (CH2OOH) 2=>2OH+2CH2O+CO	1.59E+20	-1.5	
42879.46			
IQC4H7OHTO2<=>CHOC (CH3) OHCH2Q+OH	1.20E+10	0.35	15700
CHOC (CH3) OHCH2Q=>OH+CH2O+H+CH3COCHO	1.59E+20	-1.5	
42879.46			
CH3COCHO+OH=>2CO+CH3+H2O	61329.94775	2.65419	-
4586.39996			
! REF: MIYOSHI A., IJCK, 2012, 44, 59-74			
TQC4H7OHI+O2<=>TQC4H7OHIQ2	3.49E+14	-0.816	-536.49
IQC4H7OHT+O2<=>IQC4H7OHTO2	6.87E+16	-1.627	198.7

! H-ABSTRACTION FROM ISO-BUTENOL

!REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION

SC4H7OH-I+H<=>SC4H7OH-IP+H2	7.29E+05	2.455	4361.2
SC4H7OH-I+O<=>SC4H7OH-IP+OH	1.05E+12	0.700	5884.0
SC4H7OH-I+OH<=>SC4H7OH-IP+H2O	43950.16898	2.67841	-827.103
SC4H7OH-I+HO2<=>SC4H7OH-IP+H2O2	2.92E-01	4.12	12802.0
SC4H7OH-I+CH3<=>SC4H7OH-IP+CH4	4.420E+000	3.500	5675.0
SC4H7OH-I+CH3O<=>SC4H7OH-IP+CH3OH	1.68E+11	0.000	2600.0
SC4H7OH-I+CH3O2<=>SC4H7OH-IP+CH3O2H	1.928E+004	2.600	13910.0

! BUTENOL RADICAL DECOMPOSITION

! C. ZHOU ESTIMATED

SC4H7OH-IP+H=>CH3+C3H4-A+OH	40209.73013	2.51815	8847.53569
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! KETO-ENOL ISOMERIZATIONS

SC4H7OH-I+HO2<=>IC3H7CHO+HO2	1.490E+05	1.67	6.810E+03
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! FORMIC ACID CATALYZED KETO-ENOL ISOMERIZATION

SC4H7OH-I+HOCHO=IC3H7CHO+HOCHO	2.81E-02	3.286	-4509
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! TAUTOMERIZATION OF 1-PROPENOL (CH3CHCHOH) TO PROPANAL (C2H5CHO)

!

SC4H7OH-I<=>IC3H7CHO	8.59E+11	0.318	5.59E4
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! REF: ANALOGY TO ALPHA-POSITION ABSTRACTION BY OH AND HO2 FROM N-BUTANOL

! REF: C ZHOU, ET AL. COMBUST & FLAME, 2011, 158, 726.

IC4H7OH+OH<=>IC4H6OH+H2O	1.26E+03	2.97	
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-2660.593

! REF: C ZHOU, ET AL. IJCK, 2012, 44, 155.

IC4H7OH+HO2<=>IC4H6OH+H2O2	1.45E-05	5.26	
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8267.907

!REF:ANALOGY C3H5-A+X --> PRODUCTS

IC4H6OH+H2<=>IC4H7OH+H	2.160E+004	2.380	
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18990.0

!REF:

IC4H7OH+O2<=>IC4H6OH+HO2	6.000E+013	0.000	
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39900.0

!REF:RATE CONSTANT ANALOGY TO C3H5-A+CH2O (X 5)

IC4H6OH+CH2O<=>IC4H7OH+HCO	6.300E+008	1.900	
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18190.0

!REF: ANALOGY WITH C2H4

IC4H8+O<=>IC3H7+HCO	7.450E+006	1.880	
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183.0

IC4H8+O=>CH2CO+CH3+CH3	3.050E+006	1.880	
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183.0

IC4H8+O=>IC3H6CO+H+H	3.050E+006	1.880	
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183.0

IC4H8+O<=>IC4H7+OH	1.05E+12	0.700	
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5884.0

IC4H8+O<=>IC4H7-I1+OH 8959.1	1.200E+011	0.700
! REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY		
C3H4-A+CH3<=>IC4H7 8847.53569	40209.73013	2.51815
!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS		
!IC4H8+O=>CH2CO+CH3+CH3 76.0	3.330E+007	1.760
!REF:		
!IC4H8+O=>IC3H6CO+H+H 76.0	1.660E+007	1.760
!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS		
!IC4H8+O<=>IC4H7+OH 7633.0	1.206E+011	0.700
! REF: YASUNAGA, PROC. COMBUST INST., 2009, 32, 453-460.*2		
!IC4H8+O2<=>IC4H7+HO2 37800	4.8E+13	0.000
!IC4H8+O2<=>IC4H7-I1+HO2 43500	2.0E+13	0.000
! NEW FIT		
! REF: YASUNAGA, PROC. COMBUST INST., 2009, 32, 453-460.		
IC4H8+O2<=>IC4H7+HO2 37450	3.12E+13	0.00E+00
!REF: C-J CHEN AND J. W. BOZZELLI J. PHYS. CHEM. A, 2000, 104, 9715-9732.		
IC4H8+O2<=>IC4H7-I1+HO2 62270.0	2.000E+013	0.000
! USE F. GOLDSMITH ALLYL + HO2		
!IC4H7+HO2<=>IC4H8+O2 3059.98	540.441641	2.8 -
! USE F. GOLDSMITH ALLYL + HO2 * 1.5		
!IC4H7+HO2<=>IC4H8+O2 -3059.98	810.6624615	2.8
!REF: YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.		
IC4H8+CH3<=>IC4H7+CH4 10000.0	3.2E+12	0.000
IC4H8+CH3<=>IC4H7-I1+CH4 15000.0	2.0E+12	0.000
! REF:		
!IC4H8+HO2<=>IC4H9O2 21883.0	1.085E+27	-5.2916
!IC4H8+HO2<=>IC4H8O2H-T 12620.0	3.970E+011	0.000
! ALL USE DEAN'S DATA FIRST TWO 2011, SECOND TWO 2013		

IC4H9O2<=>IC4H8+HO2	1.94E+08	1.27
29600.0		
!TC4H9O2<=>IC4H8+HO2	3.66E+10	0.62
30100		

!! REF: VILLANO, S, M.; CARSTENSEN, H-H.; DEAN, A. M. J. PHYS. CHEM. A., 2013, 117, 6458.

!IC4H8+HO2<=>IC4H9O2	1.5E-1	3.41
11700		
IC4H8+HO2<=>IC4H8O2H-T	1.64E4	2.43
8300		

!REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)

IC4H8+HO2<=>IC4H7+H2O2	2.92E-01	4.12
12802.0		

!REF: C3 NUIG CALCULATION J.MENDES

IC4H8+HO2<=>IC4H7-I1+H2O2	97038.94079	2.54892
24733.17153		

!DIVIDED THE ABOVE BY A FACTOR OF 2

!IC4H8+HO2<=>IC4H7+H2O2	1.46E-01	4.12
12802.0		

!REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)

IC4H8+HO2<=>TC4H9O2	1.04E-01	3.45
4338.0		

IC4H8+HO2<=>TC4H8O2H-I	1.000E+011	0.000
0.0		

PLOG/	0.013	6.67E+14	-2.14	14188/
PLOG/	0.9869	6.25E+06	0.64	9073 /
PLOG/	9.869	7.96E+06	0.82	8771 /
PLOG/	98.69	2.05E+13	-0.82	12919/

IC4H8+HO2<=>IC4H8O+OH	1.000E+011	0.000
0.0		

PLOG/	0.013	1.18E+04	2.29	11321/
PLOG/	0.9869	5.30E+04	2.10	11797/
PLOG/	9.869	1.47E+09	0.83	14808/
PLOG/	98.69	1.96E+17	-1.45	21195/

TC4H8O2H-I<=>IC4H8O+OH	1.000E+011	0.000
0.0		

PLOG/	0.013	5.23E+17	-2.97	8215/
PLOG/	0.9869	4.39E+22	-3.90	11424/
PLOG/	9.869	4.00E+25	-4.50	13952/
PLOG/	98.69	1.21E+27	-4.66	16324/

!REF: ANOLOGY WITH C3H5-A+HO2

IC4H7+CH3O2<=>IC4H7O+CH3O	1.000E+011	0.000
0.0		

PLOG/	0.0100	3.330E+012	-0.158	-1417.0/
PLOG/	0.1000	1.660E+014	-0.642	-349.1/
PLOG/	1.0000	2.595E+017	-1.520	2379.2/
PLOG/	10.0000	9.780E+014	-0.684	3615.3/
PLOG/	100.0000	5.470E+003	2.740	1144.4/

IC4H7+CH3O2<=>IC4H7OOCH3	1.000E+011	0.000
0.0		

PLOG/	0.0100	1.910E+031	-7.230	1336.2/
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PLOG/	0.1000	6.310E+042	-10.300	5568.9/		
PLOG/	1.0000	1.030E+045	-10.600	7851.5/		
PLOG/	10.0000	2.790E+037	-7.920	6497.9/		
PLOG/	100.0000	3.400E+029	-5.280	4539.8/		
IC4H7OOCH3<=>IC4H7O+CH3O					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.490E+058	-13.900	54266.9/		
PLOG/	0.1000	1.800E+054	-12.400	54193.8/		
PLOG/	1.0000	3.360E+046	-9.810	52468.5/		
PLOG/	10.0000	2.390E+036	-6.540	49429.0/		
PLOG/	100.0000	2.560E+027	-3.610	46333.1/		

!REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325-3346

IC4H7+HO2<=>IC4H7O+OH					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.020E+013	-0.158	-1417.0/		
PLOG/	0.1000	4.980E+014	-0.642	-349.1/		
PLOG/	1.0000	7.770E+017	-1.520	2379.2/		
PLOG/	10.0000	2.930E+015	-0.684	3615.3/		
PLOG/	100.0000	1.640E+004	2.740	1144.4/		
IC4H7+HO2<=>IC4H7OOH					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.910E+031	-7.230	1336.2/		
PLOG/	0.1000	6.310E+042	-10.300	5568.9/		
PLOG/	1.0000	1.030E+045	-10.600	7851.5/		
PLOG/	10.0000	2.790E+037	-7.920	6497.9/		
PLOG/	100.0000	1.440E+032	-6.010	6053.6/		
IC4H7+HO2<=>IC3H5CHO+H2O					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.090E+000	3.010	-3421.1/		
PLOG/	0.1000	6.350E+001	2.500	-2341.4/		
PLOG/	1.0000	6.050E+005	1.390	595.1/		
PLOG/	10.0000	3.100E+005	1.590	2677.6/		
PLOG/	100.0000	5.070E-005	4.590	927.5/		
IC4H7OOH<=>IC3H5CHO+H2O					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.990E+050	-12.700	53531.9/		
PLOG/	0.1000	4.720E+047	-11.500	54360.9/		
PLOG/	1.0000	1.500E+040	-8.840	53179.2/		
PLOG/	10.0000	2.540E+028	-5.000	49919.4/		
PLOG/	100.0000	1.480E+016	-1.120	45949.3/		
IC4H7OOH<=>IC4H7O+OH					1.000E+011	0.000
0.0						
PLOG/	0.0100	1.490E+058	-13.900	54266.9/		
PLOG/	0.1000	1.800E+054	-12.400	54193.8/		
PLOG/	1.0000	3.360E+046	-9.810	52468.5/		
PLOG/	10.0000	2.390E+036	-6.540	49429.0/		
PLOG/	100.0000	1.280E+027	-3.610	46333.1/		
IC4H7O<=>C3H5-T+CH2O					1.000E+011	0.000
0.0						
PLOG/	0.0010	7.260E+006	0.182	17815.5/		
PLOG/	0.0100	6.970E+016	-2.500	20878.7/		
PLOG/	0.1000	6.640E+023	-4.230	23565.0/		
PLOG/	1.0000	1.070E+026	-4.560	24622.9/		
PLOG/	10.0000	6.500E+029	-5.370	26645.0/		
PLOG/	100.0000	4.630E+031	-5.590	28915.3/		

PLOG/	1000.0000	8.520E+025	-3.610	27863.4/		
IC4H7O<=>IC3H5OCH2				1.000E+011	0.000	
0.0						
PLOG/	0.0010	3.170E+020	-4.150	12121.3/		
PLOG/	0.0100	4.790E+024	-5.030	14606.1/		
PLOG/	0.1000	1.900E+026	-5.160	16124.4/		
PLOG/	1.0000	1.510E+028	-5.400	18165.4/		
PLOG/	10.0000	2.420E+028	-5.170	19691.2/		
PLOG/	100.0000	5.570E+024	-3.860	19395.2/		
PLOG/	1000.0000	1.350E+018	-1.730	17386.5/		
IC4H7O<=>IC3H6CHO				1.000E+011	0.000	
0.0						
PLOG/	0.0010	5.250E-049	15.500	-15639.9/		
PLOG/	0.0100	1.460E-088	27.600	-35995.0/		
PLOG/	0.1000	4.440E-022	8.380	-3819.0/		
PLOG/	1.0000	6.230E+012	-1.440	10829.2/		
PLOG/	10.0000	3.480E+042	-9.910	25297.9/		
PLOG/	100.0000	1.880E+038	-8.160	25974.5/		
PLOG/	1000.0000	1.670E+021	-2.740	20337.7/		
IC4H7O<=>IC3H5CHO+H				1.000E+011	0.000	
0.0						
PLOG/	0.0010	3.000E+015	-2.310	14667.9/		
PLOG/	0.0100	1.500E+022	-3.960	18283.0/		
PLOG/	0.1000	1.950E+023	-3.990	19143.3/		
PLOG/	1.0000	1.150E+025	-4.240	20311.2/		
PLOG/	10.0000	1.760E+028	-4.890	22765.2/		
PLOG/	100.0000	1.410E+027	-4.280	23770.6/		
PLOG/	1000.0000	2.570E+020	-2.060	22040.1/		
IC4H7O<=>C3H6+HCO				1.000E+011	0.000	
0.0						
PLOG/	0.0010	6.620E+016	-2.840	13197.0/		
PLOG/	0.0100	1.260E+020	-3.530	15469.2/		
PLOG/	0.1000	2.130E+021	-3.640	16584.5/		
PLOG/	1.0000	1.070E+024	-4.160	18985.0/		
PLOG/	10.0000	8.420E+025	-4.400	22382.6/		
PLOG/	100.0000	1.860E+021	-2.730	23658.8/		
PLOG/	1000.0000	4.750E+008	1.140	20922.5/		
IC3H5OCH2<=>C3H5-T+CH2O				1.000E+011	0.000	
0.0						
PLOG/	0.0010	3.300E+009	-0.638	19747.8/		
PLOG/	0.0100	3.360E+021	-3.900	23945.2/		
PLOG/	0.1000	2.910E+029	-5.900	27249.7/		
PLOG/	1.0000	1.830E+034	-6.940	30690.4/		
PLOG/	10.0000	9.720E+033	-6.500	33002.5/		
PLOG/	100.0000	2.680E+027	-4.260	33305.6/		
PLOG/	1000.0000	8.810E+014	-0.326	31553.1/		
IC3H5OCH2<=>IC3H6CHO				1.000E+011	0.000	
0.0						
PLOG/	0.0010	8.010E-092	27.800	-37321.2/		
PLOG/	0.0100	7.780E-011	3.700	-2766.9/		
PLOG/	0.1000	5.110E+015	-2.760	15937.6/		
PLOG/	1.0000	4.480E+025	-5.200	21532.2/		
PLOG/	10.0000	3.970E+034	-7.410	28116.9/		
PLOG/	100.0000	5.620E+022	-3.560	25806.7/		
PLOG/	1000.0000	2.510E+020	-2.630	29288.4/		
IC3H5OCH2<=>IC3H5CHO+H				1.000E+011	0.000	
0.0						
PLOG/	0.0010	4.930E+024	-5.050	20108.4/		

PLOG/	0.0100	2.140E+028	-5.800	22219.4/		
PLOG/	0.1000	1.930E+032	-6.640	25108.2/		
PLOG/	1.0000	8.600E+034	-7.110	28209.1/		
PLOG/	10.0000	2.170E+034	-6.640	30647.6/		
PLOG/	100.0000	4.170E+028	-4.710	31231.9/		
PLOG/	1000.0000	3.980E+018	-1.620	30129.8/		
IC3H5OCH2<=>C3H6+HCO				1.000E+011		0.000
0.0						
PLOG/	0.0010	8.230E+026	-5.840	19356.9/		
PLOG/	0.0100	1.320E+029	-6.210	21293.6/		
PLOG/	0.1000	3.470E+032	-6.960	24197.3/		
PLOG/	1.0000	1.440E+036	-7.760	28007.8/		
PLOG/	10.0000	9.720E+037	-8.020	32394.6/		
PLOG/	100.0000	2.430E+031	-5.810	34295.8/		
PLOG/	1000.0000	3.730E+014	-0.726	32008.3/		
IC3H6CHO<=>C3H5-T+CH2O				1.000E+011		0.000
0.0						
PLOG/	0.0010	6.890E-069	21.500	2638.0/		
PLOG/	0.0100	5.340E-033	11.100	16749.1/		
PLOG/	0.1000	6.110E+026	-6.010	44116.7/		
PLOG/	1.0000	8.040E+035	-8.310	46919.7/		
PLOG/	10.0000	5.520E+040	-9.190	50508.7/		
PLOG/	100.0000	5.850E+035	-7.180	52038.4/		
PLOG/	1000.0000	1.930E+019	-1.940	48440.0/		
IC3H6CHO<=>IC3H5CHO+H				1.000E+011		0.000
0.0						
PLOG/	0.0010	1.610E+010	-1.240	32371.3/		
PLOG/	0.0100	5.840E+015	-2.610	32878.4/		
PLOG/	0.1000	3.640E+023	-4.600	34275.3/		
PLOG/	1.0000	7.580E+031	-6.630	37895.4/		
PLOG/	10.0000	2.860E+032	-6.300	39990.7/		
PLOG/	100.0000	1.570E+023	-3.140	38011.7/		
PLOG/	1000.0000	4.520E+012	0.214	34570.5/		
IC3H6CHO<=>C3H6+HCO				1.000E+011		0.000
0.0						
PLOG/	0.0010	2.900E+032	-7.240	25687.5/		
PLOG/	0.0100	5.300E+033	-7.280	27100.6/		
PLOG/	0.1000	2.000E+035	-7.410	29027.3/		
PLOG/	1.0000	1.010E+034	-6.700	30018.1/		
PLOG/	10.0000	9.760E+027	-4.630	28923.9/		
PLOG/	100.0000	2.110E+019	-1.850	26239.8/		
PLOG/	1000.0000	1.590E+013	0.063	24086.3/		
C3H5-T+CH2O<=>IC3H5CHO+H				1.000E+011		0.000
0.0						
PLOG/	0.0010	2.600E+004	2.260	1510.3/		
PLOG/	0.0100	5.130E+004	2.170	1675.5/		
PLOG/	0.1000	3.990E+005	1.910	2218.3/		
PLOG/	1.0000	1.750E+007	1.450	3428.0/		
PLOG/	10.0000	1.350E+009	0.933	5173.0/		
PLOG/	100.0000	2.240E+011	0.357	8001.3/		
PLOG/	1000.0000	6.010E+005	2.090	7895.6/		
C3H5-T+CH2O<=>C3H6+HCO				1.000E+011		0.000
0.0						
PLOG/	0.0010	1.110E+007	1.090	1807.2/		
PLOG/	0.0100	2.470E+007	0.993	1994.9/		
PLOG/	0.1000	2.470E+008	0.704	2596.2/		
PLOG/	1.0000	1.420E+010	0.209	3934.2/		
PLOG/	10.0000	3.450E+013	-0.726	6944.3/		

PLOG/ 100.0000 3.310E+014 -0.866 10965.7/
PLOG/ 1000.0000 1.650E+001 3.170 9399.8/

!REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732.

! HIGH PRESSURE LIMIT ONLY

IC4H7+O2<=>IC4H7O2 2290	1.09E+010	0.56725		
IC4H7O2<=>IC4H7O+O 60620	1.82E+014	0.0		
IC4H7O2<=>IC3H5CHO+OH 39460	1.52E+009	1.02524		
IC4H7O2<=>IC4H6OOH-I 19820	1.41E+005	1.83586		
IC4H6OOH-I<=>C*CYCCOC+OH 42140	6.82E+012	-0.34545		
IC4H6OOH-I<=>C3H4-A+CH2O2H 51390	1.18E+012	0.91203		
IC4H6OOH-I<=>IC3H5CHO+OH 54090	2.42E+009	0.87390		
IC4H7O2<=>CCYCCOOC-T1 28020	1.19E+008	0.80412		
CCYCCOOC-T1<=>CCYCCOOC-I2 38820	3.56E+013	0.0		
CCYCCOOC-I2<=>CHOIC3H6O 3000	3.19E+014	0.0		
CHOIC3H6O<=>CH3CHCHO+CH2O 9780	4.30E+012	0.0		
CCYCCOOC-T1<=>CCY(C2O)CO 17470	4.56E+011	0.92729		
CCY(C2O)CO<=>CCYCCO-T1+CH2O 18150	1.74E+013	0.0		
IC4H7O2<=>C2CYCOOC-I1 29720	1.07E+008	0.89161		
C2CYCOOC-I1<=>IC3H5OOCH2 18500	4.41E+013	-0.22618		
IC3H5OOCH2<=>CH3COCH2+CH2O 1000	1.41E+010	0.0		
C2CYCOOC-I1<=>CCY(C2O)CO 20320	1.21E+013	0.10180		
! IC4H6OOH-I+O2<=>O2IC4H6OOH-I 2290	1.09E+010	0.56725		
! O2IC4H6OOH-I<=>HO2IC3H4CHO 18580	4.00E+010	0.0		
! HO2IC3H4CHO<=>OIC3H4CHO+OH 40500	2.00E+016	0.0		
! IC4H8+HO2<=>IC4H7+H2O2 DIVIDED BY 2 IC4H7O2+IC4H8<=>IC4H7+IC4H7OOH 12802.0	1.46E-01	4.12		
! ANALOGY TO IC4H7+HO2 DIVIDED 4 IC4H7O2+IC4H7<=>IC4H7O+IC4H7O 0.000 0.0			1.000E+011	
PLOG/ 0.0100 2.55E+12 -0.158 -1417.0/				
PLOG/ 0.1000 1.25E+14 -0.642 -349.1/				
PLOG/ 1.0000 1.94E+17 -1.520 2379.2/				

PLOG/	10.0000	7.33E+14	-0.684	3615.3/	
PLOG/	100.0000	4.10E+03	2.740	1144.4/	
IC4H7O2+IC4H7<=>IC4H7OOIC4H7					1.000E+011
0.000	0.0				
PLOG/	0.0100	4.78E+30	-7.230	1336.2/	
PLOG/	0.1000	1.58E+42	-10.300	5568.9/	
PLOG/	1.0000	2.58E+44	-10.600	7851.5/	
PLOG/	10.0000	6.98E+36	-7.920	6497.9/	
PLOG/	100.0000	3.60E+31	-6.010	6053.6/	
IC4H7OOIC4H7<=>IC4H7O+IC4H7O					1.000E+011
0.000	0.0				
PLOG/	0.0100	3.73E+57	-13.900	54266.9/	
PLOG/	0.1000	4.50E+53	-12.400	54193.8/	
PLOG/	1.0000	8.40E+45	-9.810	52468.5/	
PLOG/	10.0000	5.98E+35	-6.540	49429.0/	
PLOG/	100.0000	3.20E+26	-3.610	46333.1/	
! ALKANES ESTIMATED					
TC4H9O2+IC4H7<=>TC4H9O+IC4H7O					7.000E+012 0.000
-1000.0					
IC4H7O2+IC4H7O2<=>IC4H7O+IC4H7O+O2					1.40E+16 -1.61
1860.0					
!IC4H7O2+IC4H7<=>IC4H7O+IC4H7O					9.000E+12 0.000 -
1000.0					
!! ANALOGY TO IC4H7+HO2 DIVIDED BY 1.3					
!TC4H9O2+IC4H7<=>TC4H9O+IC4H7O					1.000E+011
0.000	0.0				
!PLOG/	0.0100	7.85E+12	-0.158	-1417.0/	
!PLOG/	0.1000	3.83E+14	-0.642	-349.1/	
!PLOG/	1.0000	5.98E+17	-1.520	2379.2/	
!PLOG/	10.0000	2.25E+15	-0.684	3615.3/	
!PLOG/	100.0000	1.26E+04	2.740	1144.4/	
!ANALOGY WITH C3H5-A+CH3					
IC4H7+CH3 (+M) <=>AC5H10 (+M)					1.000E+014 -0.320
-262.3					
LOW/					3.910E+060 -12.810
6250.0/					
TROE/	1.040E-001	1.606E+003	6.000E+004	6.118E+003/	
H2/	2.00/	H2O/ 6.00/	CH4/ 2.00/	CO/ 1.50/	CO2/ 2.00/
C2H6/	3.00/	AR/			
0.70/					
!ANALOGY WITH C3H5-A+CH3 MULTIPLY 3 TO MATCH JSR					
!IC4H7+CH3 (+M) <=>AC5H10 (+M)					3.000E+014 -0.320
-262.3					
!LOW/					1.17E+061 -12.810
6250.0/					
!TROE/	1.040E-001	1.606E+003	6.000E+004	6.118E+003/	
!H2/	2.00/	H2O/ 6.00/	CH4/ 2.00/	CO/ 1.50/	CO2/ 2.00/
C2H6/	3.00/	AR/			
0.70/					
!!REF: FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4750-4761					
!IC4H7+IC4H7<=>H15DE25DM					1.000E+011 0.000
0.0					
!PLOG/	0.039	6.54954E+64	-15.935	20230/	

!PLOG/	0.078	1.50041E+60	-14.49	18600/	
!PLOG/	0.156	2.27097E+55	-12.995	16700/	
IC4H7+IC4H7<=>C3H4-A+AC5H10					9.550E+040
-9.300	12470.0				
PLOG/	1.0000	4.10E+40	-9.300	12470.0/	
PLOG/	4.0000	3.41E+32	-6.800	9180.0/	
PLOG/	10.0000	1.26E+28	-5.500	7410.0/	
! DEVIDED BY 2 OF THE ABOVE					
IC4H7+IC4H7<=>H15DE25DM				1.000E+011	0.000
0.0					
PLOG/	0.039	3.27E+64	-15.935	20230/	
PLOG/	0.078	7.50E+59	-14.49	18600/	
PLOG/	0.156	1.14E+55	-12.995	16700/	
!H15DE25DM+OH=>C3H5-T+B13DE2M+H2O					
	2.636965672	-6.0			1.79E+05
!H15DE25DM+OH=>C3H4-A+C2H4+C3H5-T+H2O					
2.46	729.44				5.064E+05
!REF: FROM LLNL C8-C16 N-ALKANES MECH					
!AC5H10+OH<=>AC5H9-A2+H2O					
	2.000	-298.0			3.120E+06
!AC5H10+H<=>AC5H9-A2+H2					
	2.500	2492.0			1.730E+05
!AC5H10+CH3<=>AC5H9-A2+CH4					
	3.500	5675.0			2.210E+00
AC5H10+O<=>AC5H9-A2+OH					
2.56		-1.130E+03			3.700E+05
AC5H10+OH<=>SC4H9+CH2O					
	0.000	4000.0			2.000E+10
AC5H10+O<=>SC4H9+HCO					
	2.340	-1050.0			7.230E+05
AC5H10+O<=>IC3H7+CH3CO					
	2.340	-1050.0			7.230E+05
AC5H10+O<=>IC4H9+HCO					
	2.340	-1050.0			7.230E+05
AC5H10<=>C3H5-T+C2H5					
	-2.409	100500.0			8.922E+24
!AC5H9-A2<=>C3H4-A+C2H5					
-1.63		5.924E+04			1.983E+20
!AC5H10+H<=>AC5H9-C+H2					
2.360		207.0			3.376E+05
!AC5H10+H<=>AC5H9-D+H2					
2.400		4471.0			1.950E+06
!AC5H10+OH<=>AC5H9-C+H2O					
2.640		-1919.0			2.764E+04
!AC5H10+OH<=>AC5H9-D+H2O					
1.610		-35.0			7.010E+07
!AC5H10+CH3<=>AC5H9-C+CH4					
3.310		4002.0			3.690E+00
!AC5H10+CH3<=>AC5H9-D+CH4					
3.460		5481.0			2.270E+00
!AC5H10+HO2<=>AC5H9-A2+H2O2					
2.600		13910.0			9.639E+03
!AC5H10+HO2<=>AC5H9-C+H2O2					
2.550		10530.0			4.820E+03

!AC5H10+HO2<=>AC5H9-D+H2O2	1.450E+04
2.600 13910.0	
AC5H10+CH3O2<=>AC5H9-A2+CH3O2H	9.639E+03
2.600 13910.0	
AC5H10+CH3O2<=>AC5H9-C+CH3O2H	4.820E+03
2.550 10530.0	
AC5H10+CH3O2<=>AC5H9-D+CH3O2H	1.450E+04
2.600 13910.0	
AC5H10+CH3O<=>AC5H9-A2+CH3OH	9.000E+01
2.950 11990.0	
AC5H10+CH3O<=>AC5H9-C+CH3OH	4.000E+01
2.900 8609.0	
AC5H10+CH3O<=>AC5H9-D+CH3OH	2.180E+11
0.000 4571.0	

!REF:-S IS ESTIMATED

H15DE25DM+H<=>H15DE25DM-S+H2	1.42E+06
2.3151654072075.955844	
H15DE25DM+H<=>H15DE25DM-A+H2	7.29E+05
2.455 4361.2	

!H15DE25DM+OH<=>H15DE25DM-S+H2O	1.79E+05
2.636965672-6.0	

!H15DE25DM+OH<=>H15DE25DM-A+H2O	5.064E+05
2.46 729.44	

H15DE25DM+HO2<=>H15DE25DM-S+H2O2	1.00E+00
3.8873668969386.357213	

H15DE25DM+HO2<=>H15DE25DM-A+H2O2	2.92E-01
4.12 12802.0	

H15DE25DM+CH3<=>H15DE25DM-S+CH4	1.00E+00
3.6490200083374.05195	

H15DE25DM+CH3<=>H15DE25DM-A+CH4	4.420E+000
3.500 5675.0	

H15DE25DM+O2<=>H15DE25DM-S+HO2	4.000E+014
0.000 38890.0	

H15DE25DM+O2<=>H15DE25DM-A+HO2	1.86E+9
1.301 40939	

H15DE25DM+O<=>H15DE25DM-S+OH	1.59243E+11
0.7 1.30E+01	

H15DE25DM+O<=>H15DE25DM-A+OH	1.05E+12
0.700 5884.0	

! DIVIDED BY A FACTOR OF 2 FROM THE ABOVE

H15DE25DM+OH<=>H15DE25DM-S+H2O	8.95E+04
2.636965672-6.0	

H15DE25DM+OH<=>H15DE25DM-A+H2O	2.53E+05
2.46 729.44	

!!REF:-S IS ESTIMATED *100

!H15DE25DM+H<=>H15DE25DM-S+H2	1.42E+08
2.3151654072075.955844	

!H15DE25DM+H<=>H15DE25DM-A+H2	7.29E+07
2.455 4361.2	

!
 !H15DE25DM+OH<=>H15DE25DM-S+H2O 1.79E+07
 2.636965672-6.0
 !H15DE25DM+OH<=>H15DE25DM-A+H2O 5.064E+07
 2.46 729.44
 !
 !H15DE25DM+HO2<=>H15DE25DM-S+H2O2 1.00E+02
 3.8873668969386.357213
 !H15DE25DM+HO2<=>H15DE25DM-A+H2O2 2.92E+01
 4.12 12802.0
 !
 !H15DE25DM+CH3<=>H15DE25DM-S+CH4 1.00E+02
 3.6490200083374.05195
 !H15DE25DM+CH3<=>H15DE25DM-A+CH4 4.420E+02
 3.500 5675.0
 !
 !H15DE25DM+O2<=>H15DE25DM-S+HO2 4.000E+016
 0.000 38890.0
 !H15DE25DM+O2<=>H15DE25DM-A+HO2 1.86E+11
 1.301 40939
 !
 !H15DE25DM+O<=>H15DE25DM-S+OH 1.59243E+13
 0.7 1.30E+01
 !H15DE25DM+O<=>H15DE25DM-A+OH 1.05E+14
 0.700 5884.0

 ! C ZHOU ESTIMATED
 C3H5-T+B13DE2M<=>H15DE25DM-S 7.07E+03 2.48
 6130
 C3H4-A+AC5H9-D<=>H15DE25DM-A 2.84E+04
 2.51815 8847.53569

 ! CURRAN IJCK, 2006, 38, 250-275.
 !AC5H9-D<=>C3H5-T+C2H4 1.22E12 0.64
 29370

 C2H3+C3H5-T<=>B13DE2M 8E+12 0.0 0.0
 H+B13DE2MJ<=>B13DE2M 1E+14 0.0 0.0

 !! ABSTRACTIONS FROM ALLYLIC -CH3 ANALOGY TO PROPENE

 !B13DE2M+HO2 <=> B13DE2MJ+H2O2 3.070E-002 4.403 13547.2
 !B13DE2M+H <=> B13DE2MJ+H2 3.644E+005 2.455 4361.2
 !B13DE2M+O2 <=> B13DE2MJ+HO2 5.960E+019 -1.670 46192.1
 !B13DE2M+CH3 <=> B13DE2MJ+CH4 2.210E+000 3.500 5675.0
 B13DE2M+CH3O2<=> B13DE2MJ+CH3O2H 7.680E-002 4.403 13547.2
 B13DE2M+OH <=> B13DE2MJ+H2O 4.460E+006 2.072 1050.8

 C2H3+C3H4-A <=>B13DE2MJ 9.45E+02 2.67 6850
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

 !! HYDROGEN ATOM ADDITIONS AND HO2 OXIDATIONS OF ALLYLIC SITES

 !B13DE2M+H <=> AC5H9-D 2.50E+11 0.51 2620
 !<INTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
 (4) (2006) 250-275.

!C2H4+C3H5-T <=> AC5H9-D 9.45E+02 2.67 6850
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!B13DE2M+H <=> AC5H9-C 4.000E+013 0.000 1300.0
 !<C4H6+H<=>C4H71-3, SUBMECHANISM
 !C4H612+CH3 <=> AC5H9-C 1.76E+04 2.48 6130
 !<EXTERNAL CH3 ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN.
 38 (4) (2006) 250-275.

!B13DE2M+H <=> B1E3M3J 4.24E+11 0.51 1230
 !<EXTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
 (4) (2006) 250-275.

!B12DE3M+H <=> B1E3M3J 4.24E+11 0.51 1230
 !<EXTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
 (4) (2006) 250-275.

!B13DE2M+H <=> CC5H9-A 2.50E+11 0.51 2620
 !<INTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
 (4) (2006) 250-275.

!C2H3+C3H6 <=> CC5H9-A 9.45E+02 2.67 6850
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!! R+HO2 = RO+OH
 !AC5H9-C+HO2 <=> AC5H9O-C+OH 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 AC5H9-C+CH3O2 <=> AC5H9O-C+CH3O 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 !CH3CHO+C3H5-T <=> AC5H9O-C 9.45E+02 2.67 6850
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!AC5H9-C+HO2 <=> B2E2M1OJ+OH 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 AC5H9-C+CH3O2 <=> B2E2M1OJ+CH3O 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 !CH2O+C4H72-2 <=> B2E2M1OJ 8.80E+03 2.48 6.1E+03
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!B1E3M3J+HO2 <=> B1E3M3OJ+OH 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 B1E3M3J+CH3O2 <=> B1E3M3OJ+CH3O 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 !C2H3+CH3COCH3 <=> B1E3M3OJ 9.45E+02 2.67 6850
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!B1E3M3J+HO2 <=> B2E3M1OJ+OH 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 B1E3M3J+CH3O2 <=> B2E3M1OJ+CH3O 7.000E+012 0.000 -1000.0
 !<C3H5-A+HO2, SUBMECHANISM
 !CH2O+IC4H7-I1 <=> B2E3M1OJ 8.80E+03 2.48 6.1E+03
 !<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
 M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!REF: ANALOGY C2H3+O2 KLIPPENSTEIN

IC4H7-I1+O2<=>CH3COCH3+HCO 3.100E+031 -5.944
 5748.4
 IC4H7-I1+O2<=>TC3H6CHO+O 5.380E+018 -2.140
 5142.9
 IC4H7-I1+O2<=>IC3H5CHO+OH 2.700E+019 -2.140
 5142.9

!!!! ADDED
 09/09/2014!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
 !!!!!

!ANALOGY TO PROPENE
 !REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
 IC4H7<=>IC4H7-I1 1.300E+055 -14.530
 73800.0
 PLOG/ 0.1000 1.300E+055 -14.530 73800.0/
 PLOG/ 1.0000 5.000E+051 -13.020 73300.0/
 PLOG/ 10.0000 9.700E+048 -11.730 73700.0/
 PLOG/ 100.0000 4.860E+044 -9.840 73400.0/

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 IC4H7-I1+H<=>C3H4-A+CH4 3.333E+012 0.000
 0.0
 !REF:LASKIN ET AL. IJCK 32 589-614 2000
 IC4H7-I1+H<=>C3H4-P+CH4 3.340E+012 0.000
 0.0
 IC4H7-I1+O<=>C3H6+HCO 6.000E+013 0.000
 0.0
 IC4H7-I1+OH=>C3H6+HCO+H 5.000E+012 0.000
 0.0
 IC4H7-I1+HO2=>C3H6+HCO+OH 2.000E+013 0.000
 0.0
 IC4H7-I1+HCO<=>IC4H8+CO 9.000E+013 0.000
 0.0
 IC4H7-I1+CH3<=>C3H4-P+C2H6 1.000E+011 0.000
 0.0

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!REF: THE SAME AS ALLYL+HO2
 H15DE25DM-A+HO2<=>H15DE25DM-AO+OH 7.000E+012
 0.000 -1000.0
 !PLOG/ 0.0100 9.04E+12 -0.14321 -1454.5492/
 !PLOG/ 0.1000 2.20E+13 -0.26143 -1327.89059/
 !PLOG/ 1.0000 1.28E+13 -0.1856 -1270.28914/
 !PLOG/ 10.0000 7.09E+06 1.66007 -4481.39345/
 !PLOG/ 100.0000 1.07E+05 2.24459 -5314.99428/
 !

!!ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250.
 H15DE2M-T+CH2O<=>H15DE25DM-AO 2.5E+010 0.00
 4786.58
 IC4H7+C3H4-A<=>H15DE2M-T 8.8E+03 2.48
 6130.0

H15DE25DM-S+HO2<=>H15DE25DM-SO+OH 7.000E+012
 0.000 -1000.0
 !PLOG/ 0.0100 9.04E+12 -0.14321 -1454.5492/
 !PLOG/ 0.1000 2.20E+13 -0.26143 -1327.89059/

!PLOG/	1.0000	1.28E+13	-0.1856	-1270.28914/	
!PLOG/	10.0000	7.09E+06	1.66007	-4481.39345/	
!PLOG/	100.0000	1.07E+05	2.24459	-5314.99428/	
!					
!ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250.					
IC3H5CHO+IC4H7<=>H15DE25DM-SO					2.5E+010
0.00	6329.74				
C3H5-T+IC4H7CHO<=>H15DE25DM-SO					2.5E+010
0.00	15526.42				
!IC4H7CHO+OH=>CH2CHO+C3H4-A+H2O					5.064E+07
2.46	729.44				
!					
!REF:					
!IC4H8<=>C3H5-T+CH3				1.920E+066	-14.220
128100.0					
!IC4H8<=>IC4H7+H				3.070E+055	-11.490
114300.0					
!IC4H8+H<=>C3H6+CH3				5.680E+033	-5.720
20000.0					
!REF:ANALOGY WITH TSANG '92: C3H6+R<=>PRODUCTS					
!IC4H8+H<=>IC4H7+H2				3.400E+005	2.500
2492.0					
!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS					
!IC4H8+O=>CH2CO+CH3+CH3				3.330E+007	1.760
76.0					
!REF:					
!IC4H8+O=>IC3H6CO+H+H				1.660E+007	1.760
76.0					
!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS					
!IC4H8+O<=>IC4H7+OH				1.206E+011	0.700
7633.0					
!REF:					
!IC4H8+CH3<=>IC4H7+CH4				4.420E+000	3.500
5675.0					
!IC4H8+HO2<=>IC4H7+H2O2				1.928E+004	2.600
13910.0					
!REF:ANALOGY WITH RH+RO2 --> R+RO2H					
IC4H8+O2CHO<=>IC4H7+HO2CHO				1.928E+004	2.600
13910.0					
!REF:					
!IC4H8+O2<=>IC4H7+HO2				6.000E+012	0.000
39900.0					
!REF:WESTBROOK AND PITZ ESTIMATE 1983					
IC4H8+C3H5-A<=>IC4H7+C3H6				7.940E+011	0.000
20500.0					
IC4H8+C3H5-S<=>IC4H7+C3H6				7.940E+011	0.000
20500.0					
IC4H8+C3H5-T<=>IC4H7+C3H6				7.940E+011	0.000
20500.0					

!IC4H8+OH<=>IC4H7+H2O -298.0	5.200E+006	2.000		
!IC4H8+O<=>IC3H7+HCO -1216.0	1.580E+007	1.760		
!REF:ANALOGY TO C3H6+CH3O2 IC4H8+CH3O2<=>IC4H7+CH3O2H 13547.2	1.54E-01	4.403		
IC4H8+CH3CO3<=>IC4H7+CH3CO3H 13547.2	1.54E-01	4.403		
!REF: ANALOGY TO C3H6+CH3O IC4H8+CH3O<=>IC4H7+CH3OH 2600.0	1.68E+11	0.000		
!!REF:BALDWIN, R. R., DEAN, C. E., AND WALKER, R. W., JCS FARADAY 2, 82, 1445 (1986) !IC4H8+HO2<=>IC4H8O+OH 13340.0	1.290E+012	0.000		
!!!REF:ANOLOGY WITH C3H5-A+O2 IJCK 32 589-614 2000 !IC4H7+O2=>C3H4-A+CH2O+OH 22428.0	4.990E+015	-1.400		
!PLOG/ 1.0000 4.990E+015 -1.400 22428.0/				
!PLOG/ 10.0000 2.180E+021 -2.850 30755.0/				
!IC4H7+O2<=>CH3COCH2+CH2O 20128.0	1.190E+015	-1.010		
!PLOG/ 1.0000 1.190E+015 -1.010 20128.0/				
!PLOG/ 10.0000 7.140E+015 -1.210 21046.0/				
!IC4H7+O2<=>IC3H5CHO+OH 22859.0	1.820E+013	-0.410		
!PLOG/ 1.0000 1.820E+013 -0.410 22859.0/				
!PLOG/ 10.0000 2.470E+013 -0.450 23017.0/				
! !REF: IC4H7+O<=>IC3H5CHO+H 0.0	6.030E+013	0.000		
!IC4H7<=>C3H4-A+CH3 74260.0	1.230E+047	-9.740		
!CH3O2+IC4H7<=>CH3O+IC4H7O -1000.0	7.000E+012	0.000		
!IC4H7+HO2<=>IC4H7O+OH -1000.0	7.000E+012	0.000		
!C3H5-T+CH2O<=>IC4H7O 12600.0	1.000E+011	0.000		
!REF:EA<=>8.6+7 (RING STRAIN+EABS OF PRIMARY H BY RO) IC4H7O<=>IC4H6OH 15600.0	1.391E+011	0.000		
!IC4H7O<=>IC3H5CHO+H 29100.0	5.000E+013	0.000		
!REF:CURRAN ESTIMATE IC4H6OH+IC4H8<=>IC4H7OH+IC4H7 19840.0	4.700E+002	3.300		
IC4H6OH+H<=>IC4H7OH 0.0	1.000E+014	0.000		

C3H4-A+CH2OH<=>IC4H6OH 9200.0	1.000E+011	0.000
!REF:FROM BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21, 411--429, 1992		
IC4H7O+O2<=>IC3H5CHO+HO2 1649.0	3.000E+010	0.000
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
!REF:ANALOGY CH3O+X --> CH2O+HX		
IC4H7O+HO2<=>IC3H5CHO+H2O2 0.0	3.000E+011	0.000
IC4H7O+CH3<=>IC3H5CHO+CH4 0.0	2.400E+013	0.000
IC4H7O+O<=>IC3H5CHO+OH 0.0	6.000E+012	0.000
IC4H7O+OH<=>IC3H5CHO+H2O 0.0	1.810E+013	0.000
IC4H7O+H<=>IC3H5CHO+H2 0.0	1.990E+013	0.000
!!REF:CURRAN ESTIMATE		
!IC3H5CHO+OH<=>IC3H5CO+H2O -340.0	2.690E+010	0.760
!REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.		
!IC3H5CHO+OH<=>IC3H5CO+H2O 4586.4	61329.9	2.65 -
!!REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104. MULTIPLY BY 2		
!IC3H5CHO+OH<=>IC3H5CO+H2O 4586.4	122659.9	2.65 -
!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
!IC3H5CHO+HO2<=>IC3H5CO+H2O2 11920.0	1.000E+012	0.000
!IC3H5CHO+CH3<=>IC3H5CO+CH4 8700.0	3.980E+012	0.000
IC3H5CHO+O<=>IC3H5CO+OH 1389.0	7.180E+012	0.000
!REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.		
IC3H5CHO+HO2<=>IC3H5CO+H2O2 3684.27444	1.1773E-4	4.91966
IC3H5CHO+CH3<=>IC3H5CO+CH4 4328.93484	1.24879	3.63386
!REF:		
IC3H5CHO+O2<=>IC3H5CO+HO2 40700.0	2.000E+013	0.000
!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
!IC3H5CHO+H<=>IC3H5CO+H2 2600.0	2.600E+012	0.000
IC3H5CO<=>C3H5-T+CO 34460.0	1.278E+020	-1.890

!REF: !REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
 IC3H5CHO+H<=>IC3H5CO+H2 714740.3558 2.35674
 1577.16272

!REF: ANALOGY TO ALLYL RADICAL IN C3H6
 IC3H5CHO+OH<=>IC3H4CHO-A+H2O 4.46E+06 2.072
 1050.8
 IC3H5CHO+O<=>IC3H4CHO-A+OH 5.24E+11 0.7
 5884
 IC3H5CHO+HO2<=>IC3H4CHO-A+H2O2 3.07E-02 4.403
 13547.2
 IC3H5CHO+CH3<=>IC3H4CHO-A+CH4 2.21E+00 3.5
 5675
 IC3H5CHO+O2<=>IC3H4CHO-A+HO2 5.96E+19 -1.67
 46192.1
 IC3H5CHO+H<=>IC3H4CHO-A+H2 3.64E+05 2.455
 4361.2

! REF: ANALOGY TO C3H4-A+CH3--->IC4H7 ZHOU CALCULATED AT
 QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY
 C3H4-A+HCO<=>IC3H4CHO-A 40209.73013 2.51815
 8847.53569

!REF:ANALOGY WITH C3H5-A+CH3 --> 1-C4H8 TSANG 91 (PROPENE).
 TC3H6OCHO+OH<=>TC3H6CHO+HO2 2.018E+017 -1.200
 21010.0

!REF:CURRAN AND GAFFURI, 1995.
 TC3H6OCHO<=>CH3COCH3+HCO 3.980E+013 0.000
 9700.0

!REF:
 IC3H5CHO+H<=>TC3H6CHO 1.300E+013 0.000
 1200.0
 IC3H6CO+H<=>TC3H6CHO 1.300E+013 0.000
 4800.0

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES
 TC3H6CHO+H2<=>IC3H7CHO+H 2.160E+005 2.380
 18990.0
 !IC4H7O+OH<=>IC4H7OOH 1.000E+011 0.000
 0.0
 IC4H7O+H<=>IC4H7OH 4.000E+013 0.000
 0.0

!REF:ANALOGY WITH IC4H9 --> IC4H8+H
 IC4H7OH+H<=>IC4H8OH 1.000E+013 0.000
 1200.0

!REF:ANALOGY WITH HCO+H2 --> CH2O+H

!REF:(TSANG/ HAMPSON 86) X 5
 IC4H7O+H2<=>IC4H7OH+H 9.050E+006 2.000
 17830.0

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!REF:CURRAN ESTIMATE
IC4H7+OH<=>IC4H7OH      3.000E+013      0.000
0.0
IC4H7OH+HCO<=>IC4H7O+CH2O  3.020E+011      0.000
18160.0
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!END OF ISOBUTENE
SUBMECHANISM!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
END
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