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! Experimental and Kinetic Modeling Study of the Pyrolysis and Oxidation of 1,5-Hexadiene: The Reactivity of Allylic Radicals and Their Role in the Formation of Aromatics

! Fuel

ELEMENTS

AR HE C N O H
END

SPECIES

AR !! InChI=1S/Ar
C !! InChI=1S/C
C10H10_4 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1,3,5-8H,2,4H2
C10H10 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-10H
C10H10_5 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-3,5,7-8H,4,6H2
C10H10_3 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-3,5-9H,4H2
C10H10_1 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-5,7H,6,8H2
C10H10_2 !! InChI=1S/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-7,9H,8H2
CPDC*CC*CCJ !! InChI=1S/C10H11/c1-2-3-4-7-10-8-5-6-9-10/h2-10H,1H2
CPD1C*CC*CCJ !! InChI=1S/C10H11/c1-2-3-4-7-10-8-5-6-9-10/h2-8H,1,9H2
CPDylC*CC*CC !! InChI=1S/C10H11/c1-2-3-4-7-10-8-5-6-9-10/h2-9H,1H3
bicyclicC10H11 !! InChI=1S/C10H11/c1-2-3-5-8-9-6-4-7-10(8)9/h2-10H,1H2
C4H5cyCCJC*CC*C !! InChI=1S/C10H11/c1-2-3-7-10-8-5-4-6-9-10/h2-10H,1H2
CPD1cy(CCJC*CC) !! InChI=1S/C10H11/c1-2-6-9(5-1)10-7-3-4-8-10/h1-5,7,9H,6,8H2
CPDcy(CCJC*CC) !! InChI=1S/C10H11/c1-2-6-9(5-1)10-7-3-4-8-10/h1-7,9-10H,8H2
MIndeneJ2 !! InChI=1S/C10H11/c1-8-4-2-5-9-6-3-7-10(8)9/h2-6,8H,7H2,1H3
MIndeneJ !! InChI=1S/C10H11/c1-8-4-2-5-9-6-3-7-10(8)9/h2-8,10H,1H3
C10H8 !! InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H
CPD*CPD !! InChI=1S/C10H8/c1-2-6-9(5-1)10-7-3-4-8-10/h1-8H
C6H5C*CC*CJ !! InChI=1S/C10H9/c1-2-3-7-10-8-5-4-6-9-10/h1-9H
Spiro45_C10H9 !! InChI=1S/C10H9/c1-2-6-10(7-3-1)8-4-5-9-10/h1-9H
tricyclicC10H9f !! InChI=1S/C10H9/c1-2-6-10-7-3-5-9(10)8(10)4-1/h1-9H
C10H9 !! InChI=1S/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-9H
CPD*cyCC*CCCJ !! InChI=1S/C10H9/c1-2-6-9(5-1)10-7-3-4-8-10/h1-3,5-8H,4H2
CPD*cyCC*CCJC !! InChI=1S/C10H9/c1-2-6-9(5-1)10-7-3-4-8-10/h1-7H,8H2
CPDcyCJC*CC*C !! InChI=1S/C10H9/c1-2-6-9(5-1)10-7-3-4-8-10/h1-9H
tricyclicC10H9 !! InChI=1S/C10H9/c1-2-7-10(6-1)8-4-3-5-9(8)10/h1-9H
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
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

C2H3Or_olef !! InChI=1S/C2H3O/c1-2-3/h3H,1H2
C2H3O1-2 !! InChI=1S/C2H3O/c1-2-3-1/h1H,2H2
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
C(*O)COJ !! InChI=1S/C2H3O2/c3-1-2-4/h1H,2H2
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
CH3CO3H !! InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3
C2H4O3 !! 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
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
O2CCHOJ !! 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
C3H3O2H !! InChI=1S/C3H4O2/c1-2-3-5-4/h1,4H,3H2
HOC*CC*O !! InChI=1S/C3H4O2/c4-2-1-3-5/h1-4H
C3H4O2 !! InChI=1S/C3H4O2/c4-2-1-3-5/h2-3H,1H2
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
C3H5Or_Olef_2 !! InChI=1S/C3H5O/c1-2-3-4/h1-2,4H,3H2
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
C2H3OCH2 !! InChI=1S/C3H5O/c1-3-4-2/h3H,1-2H2
C3H5O2r_Olef !! InChI=1S/C3H5O2/c1-2-3-5-4/h1-2,4H,3H2
C3H5O2r_Olef_1 !! 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
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
AC3H5OOH !! InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2
C3H6O2_Olef_1 !! InChI=1S/C3H6O2/c1-2-3-5-4/h2-4H,1H3
C3KET12 !! InChI=1S/C3H6O3/c1-3(2-4)6-5/h2-3,5H,1H3
C3KET21 !! InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3
C3KET13 !! InChI=1S/C3H6O3/c4-2-1-3-6-5/h2,5H,1,3H2
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
C3H6OOH2-1 !! InChI=1S/C3H7O2/c1-2-3-5-4/h2,4H,3H2,1H3
NC3H7O2 !! InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3
C3H7O2r_2 !! InChI=1S/C3H7O2/c1-2-3-5-4/h3-4H,2H2,1H3
C3H6OOH1-3 !! InChI=1S/C3H7O2/c1-2-3-5-4/h4H,1-3H2
C3H6OOH1-2 !! 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
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
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/h2-3H,1H2
 C4H4O !! InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H
 C4H4O2_olef_2 !! InChI=1S/C4H4O2/c1-2-4(6)3-5/h2-3H,1H2
 C4H4O2_olef_1 !! InChI=1S/C4H4O2/c5-3-1-2-4-6/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
 C4H5Or_olef !! InChI=1S/C4H5O/c1-2-3-4-5/h1-2,4H,3H2
 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/c1-3-4(2)5/h3H,1-2H2
 IC3H5CO !! InChI=1S/C4H5O/c1-4(2)3-5/h1H2,2H3
 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
 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_1 !! InChI=1S/C4H6O/c1-2-3-4-5/h2-5H,1H2
 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 !! InChI=1S/C4H6O/c1-3-4(2)5/h3,5H,1-2H2
 C2H3C \bar{O} CH3 !! InChI=1S/C4H6O/c1-3-4(2)5/h3H,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
 C4H6O2_olef_1 !! InChI=1S/C4H6O2/c1-2-3-4-6-5/h2-5H,1H2
 OC4H6O !! InChI=1S/C4H6O2/c5-3-1-2-4-6/h3-4H,1-2H2 ?
 C4H6O3_olef_3 !! InChI=1S/C4H6O3/c1-2-4(3-5)7-6/h2-4,6H,1H2
 C4H6O3_olef !! InChI=1S/C4H6O3/c5-3-1-2-4-7-6/h1-3,6H,4H2
 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
 C4H7Or_olef_4 !! InChI=1S/C4H7O/c1-2-3-4-5/h1-2,5H,3-4H2
 C3H6CHO-2 !! InChI=1S/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3
 C4H7Or_olef_7 !! InChI=1S/C4H7O/c1-2-3-4-5/h2-3,5H,1,4H2
 NC3H7CO !! InChI=1S/C4H7O/c1-2-3-4-5/h2-3H2,1H3
 C3H6CHO-3 !! InChI=1S/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3
 C4H7Or_olef_5 !! InChI=1S/C4H7O/c1-2-3-4-5/h3-5H,1-2H2
 C3H6CHO-1 !! InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2
 C4H7Or_olef_3 !! InChI=1S/C4H7O/c1-3-4(2)5/h1,3-5H,2H3
 CH2CH2COCH3 !! InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3
 C2H5COCH2 !! InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3
 C4H7Or_olef_2 !! 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
C4H7Or_olef_1 !! InChI=1S/C4H7O/c1-3-4(2)5/h5H,1-3H2
IC4H7O !! InChI=1S/C4H7O/c1-4(2)3-5/h1,3H2,2H3
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
C4H7O2r_olef_3 !! InChI=1S/C4H7O2/c1-2-3-4-6-5/h2,4-5H,1,3H2
C4H7O2r_olef !! InChI=1S/C4H7O2/c1-2-3-4-6-5/h2-3,5H,1,4H2
C4H7O2r_olef_1 !! InChI=1S/C4H7O2/c1-3-4(2)6-5/h3-5H,1-2H2
TC3H6OCHO !! InChI=1S/C4H7O2/c1-4(2)6-3-5/h3H,1-2H3
CH2CHOOHCOCH3 !! InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4,6H,2H2,1H3
CH3CHOOOCOCH3 !! InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3
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
C4H8O_olef_2 !! InChI=1S/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2
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
C4H8O_olef_1 !! InChI=1S/C4H8O/c1-3-4(2)5/h3-5H,1H2,2H3
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
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
IC4H7OOH !! InChI=1S/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3
TC3H6OHCHO !! InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3
C4H8O2 !! InChI=1S/C4H8O2/c1-4(6)2-3-5/h3-4,6H,2H2,1H3
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
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
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 !! InChI=1S/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3
TC4H9O !! InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3
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
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
IO2C4H8OH !! InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5H,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
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
CC*CCC !! 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
C5H3O !! InChI=1S/C5H3O/c6-5-3-1-2-4-5/h1,3-4H
C5H4O !! InChI=1S/C5H4O/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_2 !! InChI=1S/C5H6O/c1-3-5(6)4-2/h3-4H,1-2H2
C5H5OH !! InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1-6H
C5H6O2_olef_2 !! InChI=1S/C5H6O2/c1-2-5(7)3-4-6/h2,4H,1,3H2
C5H6O2_olef_1 !! InChI=1S/C5H6O2/c6-4-2-1-3-5-7/h1-2,4-5H,3H2
C5H6O2_olef !! InChI=1S/C5H6O2/c6-7-5-3-1-2-4-5/h1-6H
cy(C*CCCJC) !! InChI=1S/C5H7/c1-2-4-5-3-1/h1-2,5H,3-4H2
C5H7 !! InChI=1S/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2
CJ*CCC*C !! InChI=1S/C5H7/c1-3-5-4-2/h1,3-4H,2,5H2
C5H7r_olef !! InChI=1S/C5H7/c1-3-5-4-2/h1,3-5H,2H3
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
C*CCJCC*O !! InChI=1S/C5H7O/c1-2-3-4-5-6/h2-3,5H,1,4H2
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 !! InChI=1S/C5H7O/c1-2-3-4-5-6/h2H,1,3-4H2
C5H7Or_olef_4 !! InChI=1S/C5H7O/c1-2-3-4-5-6/h3-5H,1-2H2
C5H7Or_olef(m6) !! InChI=1S/C5H7O/c1-3-5(6)4-2/h1,3H,4H2,2H3
C5H7Or_olef_3 !! InChI=1S/C5H7O/c1-3-5(6)4-2/h3-5H,1-2H2

C5H7Or_Olef_6 !! InChI=1S/C5H7O/c1-3-5(6)4-2/h3H,1-2,4H2
C5H7Or_R5 !! InChI=1S/C5H7O/c6-5-3-1-2-4-5/h1-2,5H,3-4H2
C5H7O2r_Olef_3 !! InChI=1S/C5H7O2/c1-2-5(7)3-4-6/h2,4-5H,1,3H2
OC5H7O !! InChI=1S/C5H7O2/c6-4-2-1-3-5(4)7/h4H,1-3H2
C5H7O2r_Olef_1 !! InChI=1S/C5H7O2/c6-4-2-1-3-5-7/h1-2,5H,3-4H2
cy(C*CCCC) !! InChI=1S/C5H8/c1-2-4-5-3-1/h1-2H,3-5H2
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
C5H8O_Olef_7 !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2,4-6H,1,3H2
C*CCCC*O !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2,5H,1,3-4H2
C*CC*CCOH !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2-4,6H,1,5H2
C5H8O_Olef_3 !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2-6H,1H3
C5H8O_Olef_1 !! InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3
C5H8O_Olef_6 !! InChI=1S/C5H8O/c1-3-4-5(2)6/h3,6H,1-2,4H2
C5H8O_Olef_5 !! InChI=1S/C5H8O/c1-3-4-5(2)6/h3-4,6H,1H2,2H3
C5H8O2_Olef !! InChI=1S/C5H8O2/c1-2-3-4-5-7-6/h2,4-6H,1,3H2
C*CC*CCOOH !! InChI=1S/C5H8O2/c1-2-3-4-5-7-6/h2-4,6H,1,5H2
C*CC(OOH)C*C !! InChI=1S/C5H8O2/c1-3-5(4-2)7-6/h3-6H,1-2H2
C5H8O2_R5 !! InChI=1S/C5H8O2/c6-7-5-3-1-2-4-5/h1-2,5-6H,3-4H2
C5H8O3_Olef_3 !! InChI=1S/C5H8O3/c1-2-5(8-7)3-4-6/h2,4-5,7H,1,3H2
C5H8O3_Olef_1 !! InChI=1S/C5H8O3/c6-4-2-1-3-5-8-7/h1,3-4,7H,2,5H2
cy(CJCCCC) !! InChI=1S/C5H9/c1-2-4-5-3-1/h1H,2-5H2
C5H9r_Olef_2 !! InChI=1S/C5H9/c1-3-5-4-2/h1,3H,4-5H2,2H3
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
CC*CCJC !! 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
CC*CCCJ !! InChI=1S/C5H9/c1-3-5-4-2/h4-5H,1,3H2,2H3
C5H9Or_Olef !! InChI=1S/C5H9O/c1-3-4-5(2)6/h1,3,5-6H,4H2,2H3
TC4H8CHO !! InChI=1S/C5H9O/c1-3-5(2)4-6/h4-5H,2-3H2,1H3
C5H9O2r_Olef_7 !! InChI=1S/C5H9O2/c1-2-3-4-5-7-6/h1-2,6H,3-5H2
C5H9O2r_Olef !! InChI=1S/C5H9O2/c1-2-3-4-5-7-6/h2,5-6H,1,3-4H2
C5H9O2r_Olef_5 !! InChI=1S/C5H9O2/c1-2-3-4-5-7-6/h3-4,6H,1-2,5H2
C5H9O2r_Olef_4 !! InChI=1S/C5H9O2/c1-2-3-4-5-7-6/h3-6H,2H2,1H3
C5H9O2r_Olef_1 !! InChI=1S/C5H9O2/c1-3-4-5(2)7-6/h1,3,5-6H,4H2,2H3
C5H9O2r_Olef_2 !! InChI=1S/C5H9O2/c1-3-5(4-2)7-6/h1,3,5-6H,4H2,2H3
C5H9O2r_Olef_8 !! InChI=1S/C5H9O2/c1-3-5(4-2)7-6/h3,5-6H,1-2,4H2
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
cy(C*CCCC) !! InChI=1S/C6H10/c1-2-4-6-5-3-1/h1-2H,3-6H2 - C6H10Z#6
C6H10_Olef_1 !! InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3
C6H10_Olef_3 !! InChI=1S/C6H10/c1-3-5-6-4-2/h3-4,6H,1,5H2,2H3
C6H10 !! InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2
C6H10_Olef_6 !! InChI=1S/C6H10/c1-3-5-6-4-2/h3-6H,1-2H3
C*cy(CCCCC) !! InChI=1S/C6H10/c1-6-4-2-3-5-6/h1-5H2
C6H10_R5 !! InChI=1S/C6H10/c1-6-4-2-3-5-6/h2,4,6H,3,5H2,1H3
Ccy(CCC*CC) !! InChI=1S/C6H10/c1-6-4-2-3-5-6/h2-3,6H,4-5H2,1H3
C6H10O_Olef_4 !! InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2,4-5,7H,1,3,6H2
C*CCCC*O !! InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2,6H,1,3-5H2 - C6H10OAZ
C6H10O_Olef_6 !! InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2-3,6H,4-5H2,1H3
C6H10O_Olef_9 !! InChI=1S/C6H10O/c1-2-3-4-5-6-7/h3-4,6H,2,5H2,1H3
C6H10O_Olef_11 !! InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3
C*CCCcy(COC) !! InChI=1S/C6H10O/c1-2-3-4-6-5-7-6/h2,6H,1,3-5H2
C6H10O_Olef_22 !! InChI=1S/C6H10O/c1-2-3-4-6-5-7-6/h3-4,6H,2,5H2,1H3
C6H10O_Olef_14 !! InChI=1S/C6H10O/c1-2-3-6-4-5-7-6/h2,6H,1,3-5H2
epoxy12cy6 !! InChI=1S/C6H10O/c1-2-4-6-5(3-1)7-6/h5-6H,1-4H2 -
C6H10#6O#3

epoxy14cy6 !! InChI=1S/C6H10O/c1-2-6-4-3-5(1)7-6/h5-6H,1-4H2 -
C6H10#60#5
C6H10O_olef_25 !! InChI=1S/C6H10O/c1-2-6-4-3-5-7-6/h2,6H,1,3-5H2
C6H10O_olef_17 !! InChI=1S/C6H10O/c1-2-6-4-3-5-7-6/h3-4,6H,2,5H2,1H3
C6H10O_olef_1 !! InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3-4H,5H2,1-2H3
C*CCCC(*O)C!! InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3H,1,4-5H2,2H3
C6H10O_olef_2 !! InChI=1S/C6H10O/c1-3-4-5-6(2)7/h4-5H,3H2,1-2H3
C6H10O_olef_3 !! InChI=1S/C6H10O/c1-3-4-6-5(2)7-6/h3,5-6H,1,4H2,2H3
C6H10O_olef_12 !! InChI=1S/C6H10O/c1-3-5-6(4-2)7-5/h3,5-6H,1,4H2,2H3
C6H10O_olef!! InChI=1S/C6H10O/c1-3-5-6(7)4-2/h4H,2-3,5H2,1H3
C6H10O_olef_(m7) !! InChI=1S/C6H10O/c1-3-6-4-5(2)7-6/h3,5-6H,1,4H2,2H3
O*cy(CCCCC) !! InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-5H2 -
C6H10O#6K
C6H10O2_olef_5 !! InChI=1S/C6H10O2/c1-2-3-4-5-6-8-7/h2,4-
5,7H,1,3,6H2
C6H10O2_olef_15 !! InChI=1S/C6H10O2/c1-2-3-4-5-6-8-7/h2-5,7H,6H2,1H3
C6H10O2_olef_2 !! InChI=1S/C6H10O2/c1-3-4-5-6(2)8-7/h3-7H,1H2,2H3
C6H10O2_olef_10 !! InChI=1S/C6H10O2/c1-3-5-6(4-2)8-7/h3-4,6-7H,1-
2,5H2
C6H10O2_olef_8 !! InChI=1S/C6H10O2/c1-3-5-6(4-2)8-7/h3-7H,2H2,1H3
C6H10O2_olef_3 !! InChI=1S/C6H10O2/c1-3-6(8)4-
5(2)7/h3,5,7H,1,4H2,2H3
CC(OH)CC*CC*O !! InChI=1S/C6H10O2/c1-6(8)4-2-3-5-7/h2-3,5-
6,8H,4H2,1H3
C6H10O3_olef_15 !! InChI=1S/C6H10O3/c1-2-3-4-6(7)5-9-8/h3-
4,8H,2,5H2,1H3
C6H10O3_olef_18 !! InChI=1S/C6H10O3/c1-2-6(7)4-3-5-9-8/h2,8H,1,3-5H2
C6H10O3_olef_7 !! InChI=1S/C6H10O3/c1-2-6(7)4-3-5-9-8/h3-
4,8H,2,5H2,1H3
C6H10O3_olef_12 !! InChI=1S/C6H10O3/c1-2-6(9-8)4-3-5-7/h3-
6,8H,2H2,1H3
C6H10O3_olef_10 !! InChI=1S/C6H10O3/c1-3-5(7)6(4-2)9-
8/h3,6,8H,1,4H2,2H3
C6H10O3_olef_2 !! InChI=1S/C6H10O3/c1-3-6(7)4-5(2)9-
8/h3,5,8H,1,4H2,2H3
C6H10O3_olef_4 !! InChI=1S/C6H10O3/c1-6(9-8)4-2-3-5-7/h2-3,5-
6,8H,4H2,1H3
C6H10O3_olef_17 !! InChI=1S/C6H10O3/c7-5-3-1-2-4-6-9-
8/h1,3,5,8H,2,4,6H2
cy(CJCCCC)!! InChI=1S/C6H11/c1-2-4-6-5-3-1/h1H,2-6H2 - RC1C6H11#6
C6H11r_olef_1 !! InChI=1S/C6H11/c1-3-5-6-4-2/h3,5-6H,4H2,1-2H3
C*CCJCCC !! InChI=1S/C6H11/c1-3-5-6-4-2/h3,5H,1,4,6H2,2H3
C6H11r_olef!! InChI=1S/C6H11/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3
C6H11!! InChI=1S/C6H11/c1-3-5-6-4-2/h3-4H,1,5-6H2,2H3
C6H11r_olef_2 !! InChI=1S/C6H11/c1-3-5-6-4-2/h3-5H,6H2,1-2H3
C*CCCCJ !! InChI=1S/C6H11/c1-3-5-6-4-2/h3H,1-2,4-6H2
C6H11r_olef_4 !! InChI=1S/C6H11/c1-3-5-6-4-2/h4,6H,1,3,5H2,2H3
C6H11r_olef_7 !! InChI=1S/C6H11/c1-3-5-6-4-2/h5-6H,1,3-4H2,2H3
C*CC(C)CCJ !! InChI=1S/C6H11/c1-4-6(3)5-2/h4,6H,1-2,5H2,3H3
CJcy(CCCC)C!! InChI=1S/C6H11/c1-5-3-4-6(5)2/h5-6H,1,3-4H2,2H3
Ccy(CCCJCC)!! InChI=1S/C6H11/c1-6-4-2-3-5-6/h2,6H,3-5H2,1H3
Ccy(CJCCCC)!! InChI=1S/C6H11/c1-6-4-2-3-5-6/h4,6H,2-3,5H2,1H3
CJcy(CCCCC)!! InChI=1S/C6H11/c1-6-4-2-3-5-6/h6H,1-5H2
C6H11Or_olef_55 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,4,7H,1,3,5-6H2
C6H11Or_olef_48 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,4-5,7H,3,6H2,1H3
C*CCCCJCOH !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,5,7H,1,3-4,6H2
C6H11Or_olef_49 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,5-7H,3-4H2,1H3
C6H11Or_olef_33 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,6-7H,1,3-5H2

C6H11Or_Olef_35 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3,5,7H,4,6H2,1H3
C6H11Or_Olef_37 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3,6-7H,4-5H2,1H3
C6H11Or_Olef_32 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3,7H,1,4-6H2
C6H11Or_Olef_34 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-4,7H,5-6H2,1H3
C6H11Or_Olef_54 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3,5-7H,2,4H2,1H3
C6H11Or_Olef_40 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-4,6-7H,2,5H2,1H3
C6H11Or_Olef_42 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-4,7H,1-2,5-6H2
C6H11Or_Olef_39 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-5,7H,2,6H2,1H3
C6H11Or_Olef_44 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-5,7H,1-3,6H2
CCCC*CCOJ !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-5H,2-3,6H2,1H3
C6H11Or_Olef_46 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-7H,2-3H2,1H3
C6H11Or_Olef_52 !! InChI=1S/C6H11O/c1-2-3-4-5-6-7/h5-7H,1-4H2
C6H11Or_Olef_25 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,5,7H,4H2,1-2H3
C6H11Or_Olef_31 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,5-7H,1,4H2,2H3
C6H11Or_Olef_1 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,6-7H,1-2,4-5H2
C6H11Or_Olef_4 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,7H,1,4-5H2,2H3
C6H11Or_Olef_26 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,7H,2,4-5H2,1H3
C6H11Or_Olef_3 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-4,6-7H,1,5H2,2H3
C6H11Or_Olef_13 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-4,6-7H,2,5H2,1H3
C6H11Or_Olef_7 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-4,7H,5H2,1-2H3
C6H11Or_Olef_5 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-7H,1-2H3
C6H11Or_Olef_28 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4,7H,2-3,5H2,1H3
C6H11Or_Olef_14 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4-5,7H,3H2,1-2H3
C6H11Or_Olef_18 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4-7H,1,3H2,2H3
C6H11Or_Olef_16 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4-7H,2-3H2,1H3
C6H11Or_Olef_22 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h5,7H,1,3-4H2,2H3
C6H11Or_Olef_23 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h5,7H,2-4H2,1H3
C6H11Or_Olef_27 !! InChI=1S/C6H11O/c1-3-4-5-6(2)7/h7H,1-5H2
C*CC(OJ)CCC !! InChI=1S/C6H11O/c1-3-5-6(7)4-2/h4,6H,2-3,5H2,1H3
C*CCCJCCP !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h2,4,7H,1,3,5-6H2
C*CCCCJCP !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h2,5,7H,1,3-4,6H2
C*CCJCCCP !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h2-3,7H,1,4-6H2
C*CCCCCOJ !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h2H,1,3-6H2
C6H11O2r_20 !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h3-5,7H,2,6H2,1H3
C6H11O2r_18 !! InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h4-5H,2-3,6H2,1H3
C6H11O2r_3 !! InChI=1S/C6H11O2/c1-3-4-5-6(2)8-7/h3,5-7H,1,4H2,2H3
C6H11O2r_1 !! InChI=1S/C6H11O2/c1-3-4-5-6(2)8-7/h3,6-7H,1-2,4-5H2
C6H11O2r_1(m2) !! InChI=1S/C6H11O2/c1-3-4-5-6(2)8-7/h3,6H,1,4-5H2,2H3
C6H11O2r_4(m3) !! InChI=1S/C6H11O2/c1-3-4-5-6(2)8-7/h3-4,6-7H,1,5H2,2H3
C6H11O2r_14 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3,5-7H,1,4H2,2H3
C6H11O2r_15 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3,6-7H,1-2,4-5H2
C6H11O2r_9 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3,6H,1,4-5H2,2H3
C6H11O2r_13 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3-4,6-7H,1,5H2,2H3
C6H11O2r_22 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3-4,6-7H,2,5H2,1H3
C6H11O2r_23 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h4,6-7H,1-3,5H2
C6H11O2r_16 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h4,6H,2-3,5H2,1H3
C6H11O2r_24 !! InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h4-7H,2-3H2,1H3
C6H11O2r_4 !! InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h3,5-7H,1,4H2,2H3
C6H11O2r_R5_2 !! InChI=1S/C6H11O2/c1-5-2-3-6(4-5)8-7/h2,5-7H,3-4H2,1H3
C6H11O2r_R5_8 !! InChI=1S/C6H11O2/c1-5-2-3-6(4-5)8-7/h5-6H,2-4H2,1H3
C6H11O2r_R5_7 !! InChI=1S/C6H11O2/c1-5-2-3-6(4-5)8-7/h6-7H,2-4H2,1H3
CC(OH)CC*CCOJ !! InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h2-3,6,8H,4-5H2,1H3

C6H1102r_R5_11 !! InChI=1S/C6H1102/c7-8-5-6-3-1-2-4-6/h3,6-7H,1-2,4-5H2
C(OOJ)cy(CCCCC) !! InChI=1S/C6H1102/c7-8-5-6-3-1-2-4-6/h6H,1-5H2
HOOcy(CCCCJCC) !! InChI=1S/C6H1102/c7-8-6-4-2-1-3-5-6/h1,6-7H,2-5H2 - RC9C6H1102#6P
HOOcy(CCCJCCC) !! InChI=1S/C6H1102/c7-8-6-4-2-1-3-5-6/h2,6-7H,1,3-5H2 - RC5C6H1102#6P
HOOcy(CJCCCC) !! InChI=1S/C6H1102/c7-8-6-4-2-1-3-5-6/h4,6-7H,1-3,5H2 - RC3C6H1102#6P
JOOcy(CCCCC) !! InChI=1S/C6H1102/c7-8-6-4-2-1-3-5-6/h6H,1-5H2 - RC2C6H1102#6U
HOOcy(CCJCCCC) !! InChI=1S/C6H1102/c7-8-6-4-2-1-3-5-6/h7H,1-5H2 - RC4C6H1102#6P
C6H1103r_7 !! InChI=1S/C6H1103/c1-2-3-4-6(5-7)9-8/h2,6,8H,1,3-5H2
C6H1103r_5 !! InChI=1S/C6H1103/c1-2-3-4-6(5-7)9-8/h2,6-7H,1,3-5H2
C6H1103r_32 !! InChI=1S/C6H1103/c1-2-3-4-6(5-7)9-8/h3-4,6,8H,2,5H2,1H3
C6H1103r_1 !! InChI=1S/C6H1103/c1-2-3-4-6(7)5-9-8/h2,6,8H,1,3-5H2
C6H1103r_3 !! InChI=1S/C6H1103/c1-2-3-4-6(7)5-9-8/h2,6-7H,1,3-5H2
C6H1103r_38 !! InChI=1S/C6H1103/c1-2-3-4-6(7)5-9-8/h3-4,6,8H,2,5H2,1H3
C6H1103r_47 !! InChI=1S/C6H1103/c1-2-6(7)4-3-5-9-8/h2,6,8H,1,3-5H2
C6H1103r_19 !! InChI=1S/C6H1103/c1-2-6(7)4-3-5-9-8/h3-4,6,8H,2,5H2,1H3
C6H1103r_46 !! InChI=1S/C6H1103/c1-2-6(9-8)4-3-5-7/h2,6,8H,1,3-5H2
C6H1103r_28 !! InChI=1S/C6H1103/c1-2-6(9-8)4-3-5-7/h3-4,6,8H,2,5H2,1H3
C6H1103r_20 !! InChI=1S/C6H1103/c1-3-5(7)6(4-2)9-8/h3,5-6,8H,1,4H2,2H3
C6H1103r_23 !! InChI=1S/C6H1103/c1-3-5(7)6(4-2)9-8/h4-6,8H,2-3H2,1H3
C6H1103r_7(m5) !! InChI=1S/C6H1103/c1-3-6(7)4-5(2)9-8/h3,5-6,8H,1,4H2,2H3
C6H1103r_5(m0) !! InChI=1S/C6H1103/c1-3-6(9-8)4-5(2)7/h3,5-6,8H,1,4H2,2H3
C6H1103r_13 !! InChI=1S/C6H1103/c1-6(7)4-2-3-5-9-8/h2-3,6,8H,4-5H2,1H3
C6H1103r_10 !! InChI=1S/C6H1103/c1-6(9-8)4-2-3-5-7/h2-3,6,8H,4-5H2,1H3
C6H1103r_40 !! InChI=1S/C6H1103/c7-5-3-1-2-4-6-9-8/h1,3,8H,2,4-6H2
C6H1103r_43 !! InChI=1S/C6H1103/c7-5-3-1-2-4-6-9-8/h2,4,8H,1,3,5-6H2
C6H1202_Olef_1 !! InChI=1S/C6H1202/c1-2-3-4-5-6-8-7/h4-5,7H,2-3,6H2,1H3
C6H1202_Olef_2 !! InChI=1S/C6H1202/c1-3-5-6(4-2)8-7/h4,6-7H,2-3,5H2,1H3
C6H1203_Olef_8H,1,4H2,2H3 !! InChI=1S/C6H1203/c1-3-6(9-8)4-5(2)7/h3,5-6,8H,1,4H2,2H3
C6H1203_Olef_2 !! InChI=1S/C6H1203/c1-6(7)4-2-3-5-9-8/h2-3,6-8H,4-5H2,1H3
C6H1204_Olef_18 !! InChI=1S/C6H1204/c1-2-3-4-6(10-8)5-9-7/h3-4,6-8H,2,5H2,1H3
C6H1204_Olef_20 !! InChI=1S/C6H1204/c1-2-6(10-8)4-3-5-9-7/h2,6-8H,1,3-5H2
C6H1204_Olef_15 !! InChI=1S/C6H1204/c1-2-6(10-8)4-3-5-9-7/h3-4,6-8H,2,5H2,1H3
C6H1204_Olef_12 !! InChI=1S/C6H1204/c1-3-5(9-7)6(4-2)10-8/h3,5-8H,1,4H2,2H3
C6H1204_Olef_4 !! InChI=1S/C6H1204/c1-3-6(10-8)4-5(2)9-7/h3,5-8H,1,4H2,2H3
C6H1204_Olef_2 !! InChI=1S/C6H1204/c1-6(10-8)4-2-3-5-9-7/h2-3,6-8H,4-5H2,1H3
C6H1204_Olef_23 !! InChI=1S/C6H1204/c7-9-5-3-1-2-4-6-10-8/h1,3,7-8H,2,4-6H2
C6H1304r_2 !! InChI=1S/C6H1304/c1-2-3-4-6(10-8)5-9-7/h6-7H,2-5H2,1H3
C6H1304r_7 !! InChI=1S/C6H1304/c1-2-3-6(10-8)4-5-9-7/h6,8H,2-5H2,1H3
C6H1304r_1 !! InChI=1S/C6H1304/c1-2-3-6(10-8)4-5-9-7/h6-7H,2-5H2,1H3

C6H13O4r_6 !! InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-6,8H,3-4H2,1-2H3
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
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
cy(C*CC*CCJC) !! InChI=1S/C6H7/c1-2-4-6-5-3-1/h1-5H,6H2
cy(CJC*CcyCCC) !! InChI=1S/C6H7/c1-2-5-4-6(5)3-1/h1-3,5-6H,4H2
C*cy(CCJCC*C) !! InChI=1S/C6H7/c1-6-4-2-3-5-6/h2,4-5H,1,3H2
C*cy(CCJC*CC) !! InChI=1S/C6H7/c1-6-4-2-3-5-6/h2-4H,1,5H2
Ccy(CJC*CC*C) !! InChI=1S/C6H7/c1-6-4-2-3-5-6/h2-5H,1H3
CJcy(CC*CC*C) !! InChI=1S/C6H7/c1-6-4-2-3-5-6/h2-6H,1H2
C6H7Or_olef_1 !! InChI=1S/C6H7O/c1-2-3-4-5-6-7/h2,4-5H,1,3H2
C*CC*CCJ*O!! InChI=1S/C6H7O/c1-2-3-4-5-6-7/h2-4H,1,5H2
C6H7Or_olef!! InChI=1S/C6H7O/c1-2-3-4-5-6-7/h2-5H,1H3
C6H7O2r_R5_2 !! InChI=1S/C6H7O2/c1-5-2-3-6(4-5)8-7/h2-3,6H,1,4H2
C6H7O2r_olef_5 !! InChI=1S/C6H7O2/c1-5-2-3-6(4-5)8-7/h2-4,6H,1H3
C6H7O2r_R5_1 !! InChI=1S/C6H7O2/c1-5-3-2-4-6(5)8-7/h2,4,6H,1,3H2
C6H7O2r_R5 !! InChI=1S/C6H7O2/c1-5-3-2-4-6(5)8-7/h2-3,6H,1,4H2
C6H7O2r_olef_4 !! InChI=1S/C6H7O2/c1-5-3-2-4-6(5)8-7/h2-4,6H,1H3
C6H7O2r_olef_6 !! InChI=1S/C6H7O2/c1-6(8-7)4-2-3-5-6/h2-5H,1H3
C6H7O2r_olef !! InChI=1S/C6H7O2/c7-8-5-6-3-1-2-4-6/h1,3-4H,2,5H2
C6H7O2r_olef_7 !! InChI=1S/C6H7O2/c7-8-5-6-3-1-2-4-6/h1-3H,4-5H2
C6H7O2r_olef_3 !! InChI=1S/C6H7O2/c7-8-5-6-3-1-2-4-6/h1-4,6H,5H2
C6H7O2r_olef_2 !! InChI=1S/C6H7O2/c7-8-6-4-2-1-3-5-6/h1-4,6H,5H2
C6H7O2r_olef_1 !! InChI=1S/C6H7O2/c7-8-6-4-2-1-3-5-6/h2-6H,1H2
cy(C*CCC*CC) !! InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-2,5-6H,3-4H2
cy(C*CC*CCC) !! InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-4H,5-6H2
C#CCCC*C !! InChI=1S/C6H8/c1-3-5-6-4-2/h1,4H,2,5-6H2
C*C*CCC*C !! InChI=1S/C6H8/c1-3-5-6-4-2/h3,6H,1-2,5H2
C*CC*CC*C !! InChI=1S/C6H8/c1-3-5-6-4-2/h3-6H,1-2H2
Ccy(C*CCC*C) !! InChI=1S/C6H8/c1-6-4-2-3-5-6/h2,4-5H,3H2,1H3
C*cy(CC*CCC) !! InChI=1S/C6H8/c1-6-4-2-3-5-6/h2,4H,1,3,5H2
C*cy(CCC*CC) !! InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-3H,1,4-5H2
Ccy(C*CC*CC) !! InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-4H,5H2,1H3
Ccy(CC*CC*C) !! InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-6H,1H3
C6H8O_olef_15 !! InChI=1S/C6H8O/c1-2-3-4-5-6-7/h2,4-6H,1,3H2
C*CC*CCC*O !! InChI=1S/C6H8O/c1-2-3-4-5-6-7/h2-4,6H,1,5H2
C6H8O_olef_9 !! InChI=1S/C6H8O/c1-2-3-4-5-6-7/h2-6H,1H3
C6H8O_olef_7 !! InChI=1S/C6H8O/c1-2-3-4-6-5-7-6/h2-4,6H,1,5H2
C6H8O_olef_2 !! InChI=1S/C6H8O/c1-2-6-4-3-5-7-6/h2-4,6H,1,5H2
C6H8O_olef_18 !! InChI=1S/C6H8O/c1-3-4-5-6(2)7/h3-5H,1H2,2H3
C6H8O_olef !! InChI=1S/C6H8O/c1-3-5-6(4-2)7-5/h3-6H,1-2H2
C*CC(*O)CC*C !! InChI=1S/C6H8O/c1-3-5-6(7)4-2/h3-4H,1-2,5H2

C6H8O_Olef_14 !! InChI=1S/C6H8O/c1-3-5-6(7)4-2/h3-5H,2H2,1H3
C6H8O2_Olef_1 !! InChI=1S/C6H8O2/c1-2-6(8)4-3-5-7/h3-5H,2H2,1H3
C6H8O3_Olef_4 !! InChI=1S/C6H8O3/c1-2-3-4-6(5-7)9-8/h2-6,8H,1H2
C6H8O3_Olef_1 !! InChI=1S/C6H8O3/c1-2-6(7)4-3-5-9-8/h2-4,8H,1,5H2
C6H8O3_Olef_10 !! InChI=1S/C6H8O3/c1-2-6(9-8)4-3-5-7/h2-6,8H,1H2
C6H8O3_Olef_3 !! InChI=1S/C6H8O3/c1-3-5(7)6(4-2)9-8/h3-4,6,8H,1-2H2
cy(C*CCCJCC) !! InChI=1S/C6H9/c1-2-4-6-5-3-1/h1-2,5H,3-4,6H2
cy(C*CCJCCC) !! InChI=1S/C6H9/c1-2-4-6-5-3-1/h1-3H,4-6H2
CJ*CCCC*C !! InChI=1S/C6H9/c1-3-5-6-4-2/h1,3-4H,2,5-6H2
C6H9r_Olef !! InChI=1S/C6H9/c1-3-5-6-4-2/h3,5-6H,1-2,4H2
C6H9-A !! InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2
C*CCJC*CC !! InChI=1S/C6H9/c1-3-5-6-4-2/h3-6H,1H2,2H3
C*CJCCC*C !! InChI=1S/C6H9/c1-3-5-6-4-2/h3H,1-2,5-6H2
CJcy(CC*CCC) !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2,4,6H,1,3,5H2
C6H9r_R5_5 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2,4-6H,3H2,1H3
C6H9r_R5_1 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2,4H,3,5H2,1H3
C6H9r_R5 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2,5H,3-4H2,1H3
CJcy(CCC*CC) !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2-3,6H,1,4-5H2
C6H9r_R5_2 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2-3H,4-5H2,1H3
Ccy(CCJC*CC) !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2-4,6H,5H2,1H3
C6H9r_R5_7 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h2H,1,3-5H2
C6H9r_R5_10 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h4-5H,2-3H2,1H3
C6H9r_R5_9 !! InChI=1S/C6H9/c1-6-4-2-3-5-6/h4H,1-3,5H2
C*(CJ)CC*C !! InChI=1S/C6H9/c1-4-5-6(2)3/h4H,1-3,5H2
CJ*C(C)CC*C !! InChI=1S/C6H9/c1-4-5-6(2)3/h2,4H,1,5H2,3H3
C*CCC*CJC !! InChI=1S/C6H9/c1-3-5-6-4-2/h3,6H,1,5H2,2H3
C6H9Or_Olef_18 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2,4-5H,1,3,6H2
C6H9Or_Olef !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2,4-7H,1,3H2
C6H9Or_Olef_2 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-3H,4-5H2,1H3
C6H9Or_Olef_9 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-5H,6H2,1H3
C6H9Or_Olef_6 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2H,1,3-5H2
C6H9Or_Olef_3 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h3-4H,2,5H2,1H3
C6H9Or_Olef_5 !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h4-5H,2-3H2,1H3
C6H9Or_Olef_22 !! InChI=1S/C6H9O/c1-3-4-5-6(2)7/h3-6H,1H2,2H3
C6H9Or_Olef_12 !! InChI=1S/C6H9O/c1-3-5-6(7)4-2/h3-4,6H,1-2,5H2
C6H9Or_Olef_13 !! InChI=1S/C6H9O/c1-3-5-6(7)4-2/h3-6H,2H2,1H3
C6H9O2r_Olef !! InChI=1S/C6H9O2/c1-2-3-4-5-6-8-7/h2,4-5H,1,3,6H2
CPC*CCJC*C !! InChI=1S/C6H9O2/c1-2-3-4-5-6-8-7/h2-5,7H,1,6H2
C6H9O2r_Olef_11 !! InChI=1S/C6H9O2/c1-2-3-4-5-6-8-7/h2-5H,6H2,1H3
C6H9O2r_Olef_14 !! InChI=1S/C6H9O2/c1-2-3-4-6(8)5-7/h3-4H,2,5H2,1H3
C6H9O2r_Olef(m1) !! InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h2H,1,3-5H2
C6H9O2r_Olef_7 !! InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h3-4H,2,5H2,1H3
C6H9O2r_Olef_12 !! InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h3-6H,2H2,1H3
C6H9O2r_Olef_4 !! InChI=1S/C6H9O2/c1-3-4-5-6(2)8-7/h3-6H,1H2,2H3
C6H9O2r_Olef_18 !! InChI=1S/C6H9O2/c1-3-4-5-6(2)8-7/h3-7H,1-2H2
C6H9O2r_Olef_10 !! InChI=1S/C6H9O2/c1-3-5(7)6(8)4-2/h3,6H,1,4H2,2H3
C6H9O2r_Olef_15 !! InChI=1S/C6H9O2/c1-3-5-6(4-2)8-7/h3-4,6H,1-2,5H2
C6H9O2r_Olef_6 !! InChI=1S/C6H9O2/c1-3-5-6(4-2)8-7/h3-6H,2H2,1H3
C6H9O2r_Olef_16 !! InChI=1S/C6H9O2/c1-3-5-6(4-2)8-7/h3-7H,1-2H2
C6H9O2r_Olef_2 !! InChI=1S/C6H9O2/c1-3-6(8)4-5(2)7/h3,5H,1,4H2,2H3
C6H9O2r_R5_1 !! InChI=1S/C6H9O2/c1-5-2-3-6(4-5)8-7/h2-3,5-
6H,4H2,1H3
C6H9O2r_R5_2 !! InChI=1S/C6H9O2/c1-5-2-3-6(4-5)8-7/h2-3,6-
7H,4H2,1H3
C6H9O2r_R5 !! InChI=1S/C6H9O2/c1-5-3-2-4-6(5)8-7/h2,4-6H,3H2,1H3
C6H9O2r_R5_3 !! InChI=1S/C6H9O2/c1-5-3-2-4-6(5)8-7/h2,4-7H,1,3H2
C6H9O2r_R5_4 !! InChI=1S/C6H9O2/c1-5-3-2-4-6(5)8-7/h2-7H,1H3
C6H9O2r_Olef(m4) !! InChI=1S/C6H9O2/c1-6(8)4-2-3-5-7/h2-3,5-6H,4H2,1H3

C6H9O2r_Olef_17 !! InChI=1S/C6H9O2/c7-5-3-1-2-4-6-8/h1,3,5H,2,4,6H2
COOJcy(CCC*CC) !! InChI=1S/C6H9O2/c7-8-5-6-3-1-2-4-6/h1-2,6H,3-5H2
CPcy(CCJC*CC) !! InChI=1S/C6H9O2/c7-8-5-6-3-1-2-4-6/h1-3,6-7H,4-5H2
JOOcy(CCC*CCC) !! InChI=1S/C6H9O2/c7-8-6-4-2-1-3-5-6/h1-2,6H,3-5H2
HOOcy(CCC*CCJC) !! InChI=1S/C6H9O2/c7-8-6-4-2-1-3-5-6/h1-3,6-7H,4-5H2
C6H9O2r_R6 !! InChI=1S/C6H9O2/c7-8-6-4-2-1-3-5-6/h2,4,6H,1,3,5H2
C6H9O2r_R6_1 !! InChI=1S/C6H9O2/c7-8-6-4-2-1-3-5-6/h2-4,6-7H,1,5H2
C6H9O4r_Olef_13 !! InChI=1S/C6H9O4/c1-2-3-4-6(10-8)5-9-7/h2-4,6-7H,1,5H2
C6H9O4r_1 !! InChI=1S/C6H9O4/c1-2-5(8)3-6(4-7)10-9/h4,6H,2-3H2,1H3
C6H9O4r_3 !! InChI=1S/C6H9O4/c1-2-5(8)6(10-9)3-4-7/h4,6H,2-3H2,1H3
C6H9O4r_Olef_7 !! InChI=1S/C6H9O4/c1-2-6(10-8)4-3-5-9-7/h2-4,6,8H,1,5H2
C6H9O4r_Olef_10 !! InChI=1S/C6H9O4/c1-2-6(10-8)4-3-5-9-7/h2-4,6-7H,1,5H2
C6H9O4r_Olef_1 !! InChI=1S/C6H9O4/c1-3-5(9-7)6(4-2)10-8/h3-7H,1-2H2
C6H9O4r_Olef_17 !! InChI=1S/C6H9O4/c7-9-5-3-1-2-4-6-10-8/h1-4,7H,5-6H2
C7H10_R5_2 !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h2,5H,1,3-4,6H2
C7H10_R5_11 !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h2-3,5,7H,1,4,6H2
C7H10_R5_6 !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h2-3,5H,4,6H2,1H3
C*Ccy(CCC*CC) !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h2-4,7H,1,5-6H2
C7H10_R5_10 !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h2-4H,5-6H2,1H3
CCcyC*CCC*C !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h3,5-6H,2,4H2,1H3
CCcyC*CC*CC !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h3-5H,2,6H2,1H3
CCcyCC*CC*C !! InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h3-7H,2H2,1H3
C7H10_R5_5 !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h1-5H2
Ccy(C*CC(C)*CC) !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h3,5H,4H2,1-2H3
C7H10_R5_15 !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h3-4,7H,1,5H2,2H3
Ccy(C*CC*(C)C) !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h3-4H,5H2,1-2H3
Ccy(CC*(C)C*(C)) !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h3-6H,1-2H3
C7H10_R5_13 !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h4H,1,3,5H2,2H3
C7H10_R5_4 !! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h5H,1,3-4H2,2H3
C7H10_R5_1 !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h1-5H2
C7H10_R5_8 !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h3,5,7H,1,4H2,2H3
C7H10_R5_9 !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h3-4,7H,1,5H2,2H3
Ccy(C*(C)C*(C)) !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h3-4H,5H2,1-2H3
Ccy(CC(C)*CC*(C)) !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h3-6H,1-2H3
Ccy(C*CCC*(C)) !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h4-5H,3H2,1-2H3
C7H10_R5_3 !! InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h5H,1,3-4H2,2H3
Ccy(C(C)C*CC*(C)) !! InChI=1S/C7H10/c1-7(2)5-3-4-6-7/h3-6H,1-2H3
Ccy(C*CC*CCC) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,5H,4,6H2,1H3
Ccy(C*CCC*CC) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,6H,4-5H2,1H3
C*cy(CCC*CCC) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3H,1,4-6H2
Ccy(CC*CC*CC) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-5,7H,6H2,1H3
Ccy(C*CCCC*(C)) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3,5-6H,2,4H2,1H3
C7H10_R6 !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3,5H,1-2,4,6H2
Ccy(CC*CCC*(C)) !! InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3-7H,2H2,1H3
C7H11r_R5_41 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2,5,7H,1,3-4,6H2
C7H11r_R5_55 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2,5H,3-4,6H2,1H3
C7H11r_R5_32 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2-3,5,7H,4,6H2,1H3
C7H11r_R5_19 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2-3,7H,1,4-6H2
C7H11r_R5_13 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2-3H,4-6H2,1H3
C7H11r_R5_35 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2-4,7H,5-6H2,1H3
C7H11r_R5_2 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h2H,1,3-6H2
C7H11r_R5_33 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3,5,7H,1-2,4,6H2
C7H11r_R5_74 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3,5-7H,2,4H2,1H3

C7H11r_R5_7!! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3,5H,2,4,6H2,1H3
C7H11r_R5_37 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3,6H,2,4-5H2,1H3
C7H11r_R5_36 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3-4,7H,1-2,5-6H2
C7H11r_R5_38 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3-4H,2,5-6H2,1H3
C7H11r_R5_75 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h3-5,7H,2,6H2,1H3
C7H11r_R5_44 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h5-6H,2-4H2,1H3
C7H11r_R5_56 !! InChI=1S/C7H11/c1-2-7-5-3-4-6-7/h5H,1-4,6H2
C7H11r_Olef_29 !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,5,7H,1-2,4,6H2
CCC*CC*CCJ !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,5-7H,1,4H2,2H3
C7H11r_Olef_27 !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,6-7H,1-2,4-5H2
C*CCC*CCJC !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-4,6-7H,1,5H2,2H3
C*CCCCJC*C !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-5H,1-2,6-7H2
C*CCJCC*CC !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-6H,1,7H2,2H3
CC*CC*CCJC !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-7H,1-2H3
C7H11r_Olef_15 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4,6H,1,3,5H2,2H3
C7H11r_Olef_17 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4,6H,1-2,5H2,3H3
C7H11r_Olef_20 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4,6H,2-3,5H2,1H3
C7H11r_Olef_23 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-5,7H,1-3,6H2
C7H11r_Olef_14 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-5H,1,3,6H2,2H3
C7H11r_Olef!! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-5H,1-2,6H2,3H3
C7H11r_Olef_9 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-6H,1H2,2-3H3
C7H11r_Olef_3 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-6H,2H2,1,3H3
C7H11r_Olef_7 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-6H,3H2,1-2H3
C7H11r_Olef_2 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-7H,1-2H2,3H3
C7H11r_Olef_5 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-7H,2-3H2,1H3
C7H11r_Olef_18 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h4H,1-3,5-6H2
C7H11r_Olef_12 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h5-6H,1-2,4H2,3H3
C7H11r_Olef_10 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h5-6H,2-4H2,1H3
C7H11r_Olef_13 !! InChI=1S/C7H11/c1-4-6-7(3)5-2/h5H,1-4,6H2
C7H11r_R5_47 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h1,3-5H2,2H3
C7H11r_R5_48 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3,5,7H,4H2,1-2H3
C7H11r_R5_60 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3,5-6H,4H2,1-2H3
C7H11r_R5_64 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3,7H,1,4-5H2,2H3
C7H11r_R5_63 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3-4,6-
7H,1,5H2,2H3
C7H11r_R5_50 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3-4,6H,5H2,1-2H3
C7H11r_R5_51 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3-7H,1-2H3
C7H11r_R5_57 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h3H,4-5H2,1-2H3
C7H11r_R5_20 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h4,6H,1,3,5H2,2H3
C7H11r_R5_59 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h4,7H,1,3,5H2,2H3
C7H11r_R5_8!! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h5,7H,1,3-4H2,2H3
C7H11r_R5_12 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h5-6H,1,3-4H2,2H3
C7H11r_R5_46 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h5H,3-4H2,1-2H3
C7H11r_R5_11 !! InChI=1S/C7H11/c1-6-3-4-7(2)5-6/h6H,1-5H2
C7H11r_R5_54 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h1,3-5H2,2H3
C7H11r_R5_17 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3,5-7H,1,4H2,2H3
C7H11r_R5_16 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3,7H,1,4-5H2,2H3
C7H11r_R5_27 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3-4,6-
7H,1,5H2,2H3
C7H11r_R5_25 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3-4,6H,5H2,1-2H3
C7H11r_R5_6!! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3-4,7H,5H2,1-2H3
C7H11r_R5_73 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3-7H,1-2H3
C7H11r_R5_24 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h3H,4-5H2,1-2H3
C7H11r_R5_28 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h4,7H,1,3,5H2,2H3
C7H11r_R5_52 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h4-6H,3H2,1-2H3
C7H11r_R5_23 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h4H,3,5H2,1-2H3
C7H11r_R5_43 !! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h5,7H,1,3-4H2,2H3
C7H11r_R5_5!! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h5-6H,1,3-4H2,2H3

C7H11r_R5_3!! InChI=1S/C7H11/c1-6-4-3-5-7(6)2/h6H,1-5H2
Ccy(C*CCCJCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2,5H,3-4,6H2,1H3
Ccy(CCJC*CCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-
3,5,7H,4,6H2,1H3
Ccy(CCJCC*CC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3,6-7H,4-
5H2,1H3
CJcy(CCC*CCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3,7H,1,4-6H2
Ccy(CJCC*CCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3H,4-6H2,1H3
Ccy(CCC*CCJC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-4,7H,5-6H2,1H3
C*cy(CCCCJCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2H,1,3-6H2
CJcy(CC*CCCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5,7H,1-2,4,6H2
Ccy(CC*CCCCJ) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5-7H,2,4H2,1H3
Ccy(CJC*CCCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5H,2,4,6H2,1H3
Ccy(C*CCCCJC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,6H,2,4-5H2,1H3
Ccy(CC*CCCJC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3-5,7H,2,6H2,1H3
C*cy(CCCJCCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3H,1-2,4-6H2
Ccy(C*CCCCCJ) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h5-6H,2-4H2,1H3
CJcy(C*CCCC) !! InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h5H,1-4,6H2
C*cy(CCCCC) !! InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h1-6H2
Ccy(CCC*CCC) !! InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h2-3,7H,4-6H2,1H3
Ccy(CC*CCCC) !! InChI=1S/C7H12/c1-7-5-3-2-4-6-
7/h3,5,7H,2,4,6H2,1H3
Ccy(C*CCCC) !! InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3
Ccy(CCCCJCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h2,7H,3-6H2,1H3
Ccy(CJCCCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h2-6H2,1H3
Ccy(CCCJCCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h3,7H,2,4-6H2,1H3
Ccy(CCJCCCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h5,7H,2-4,6H2,1H3
CJcy(CCCCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h7H,1-6H2
C*CCCC*CC !! InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4,6H,1,5,7H2,2H3
C*(C)CCC*C !! InChI=1S/C7H12/c1-4-5-6-7(2)3/h4H,1-2,5-6H2,3H3
C*CC(C)CC*C !! InChI=1S/C7H12/c1-4-6-7(3)5-2/h4-5,7H,1-2,6H2,3H3
C*CCCCJCC !! InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,6H,1,4-5,7H2,2H3
C*CCCC(C)CJ !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h4,7H,1-2,5-6H2,3H3
C*CCJCC(C)C !! InChI=1S/C7H13/c1-4-5-6-7(2)3/h4-5,7H,1,6H2,2-3H3
C*CCC(C)CJC !! InChI=1S/C7H13/c1-4-6-7(3)5-2/h4-5,7H,1,6H2,2-3H3
C*CCC(C)CCJ !! InChI=1S/C7H13/c1-4-6-7(3)5-2/h4,7H,1-2,5-6H2,3H3
CCJCC(C)*C !! InChI=1S/C7H13/c1-4-6-7(3)5-2/h4-5,7H,2,6H2,1,3H3
C*CCCCJCC !! InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,6H,1,4-5,7H2,2H3
CJCCCC*CC !! InChI=1S/C7H13/c1-3-5-7-6-4-2/h4,6H,1,3,5,7H2,2H3
CC*CCCCJC !! InChI=1S/C7H13/c1-3-5-7-6-4-2/h3-5H,6-7H2,1-2H3
Ccy(CCJCCCC) !! InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h5,7H,2-4,6H2,1H3
CCJCCCC*C !! InChI=1S/C7H13/c1-3-5-7-6-4-2/h3-4H,1,5-7H2,2H3
C*CC(C)CCCJ !! InChI=1S/C7H13/c1-4-6-7(3)5-2/h5,7H,1-2,4,6H2,3H3
C7H7 !! InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-6H,1H2
C*CcyCC*CC*C !! InChI=1S/C7H8/c1-2-7-5-3-4-6-7/h2-7H,1H2
C*CcyC*CC*CC !! InChI=1S/C7H8/c1-2-7-5-3-4-6-7/h2-5H,1,6H2
C*CcyC*CCC*C !! InChI=1S/C7H8/c1-2-7-5-3-4-6-7/h2-3,5-6H,1,4H2
C*cy(CC*CC*CC) !! InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-5H,1,6H2
C7H8 !! InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
C*cy(CC*CCC*C) !! InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h3-6H,1-2H2
C7H9r_R5_7 !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2,5-6H,1,3-4H2
CC*cy(CCJCC*C) !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-3,5-6H,4H2,1H3
C7H9r_R5_21 !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-3,5-7H,1,4H2
C7H9r_R5_5 !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-3,5H,1,4,6H2
C*Ccy(C*CCCJC) !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-3,6H,1,4-5H2
C7H9r_R5_17 !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-4H,1,5-6H2
C7H9r_R5_18 !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-5,7H,1,6H2
CC*cy(CCJC*CC) !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-5H,6H2,1H3

CCJcyCC*CC*C !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h2-7H,1H3
 CJCcyC*CCC*C !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h3,5-6H,1-2,4H2
 CJCcyC*CC*CC !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h3-5H,1-2,6H2
 CCcyCJC*CC*C !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h3-6H,2H2,1H3
 CJCcyCC*CC*C !! InChI=1S/C7H9/c1-2-7-5-3-4-6-7/h3-7H,1-2H2
 C*C*CCCJC*C!! InChI=1S/C7H9/c1-3-5-7-6-4-2/h3,5-6H,1-2,7H2
 bicyclicC7H9 !! InChI=1S/C7H9/c1-5-6-3-2-4-7(5)6/h2-7H,1H3
 C7H9r_Olef_5 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3,5H,1,4H2,2H3
 C7H9r_R5_25!! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-4,6H,1-2,5H2
 C7H9r_R5_22!! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-4H,1,5H2,2H3
 C7H9r_Olef_2 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-5,7H,1H2,2H3
 C7H9r_Olef_4 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-5H,1-2H3
 C7H9r_Olef_3 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-6H,1H2,2H3
 C7H9r_R5_10!! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3H,1-2,4-5H2
 C7H9r_Olef_6 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h4-5H,1,3H2,2H3
 C7H9r_R5_9 !! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h5H,1-4H2
 C7H9r_R5_2 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3,5H,1,4H2,2H3
 C7H9r_R5_12!! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-4,6H,1-2,5H2
 C7H9r_R5_16!! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-4,7H,1-2,5H2
 C7H9r_R5_15!! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-4H,1,5H2,2H3
 C7H9r_R5_1 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-5,7H,1H2,2H3
 C7H9r_Olef_12 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-5H,1-2H3
 C7H9r_Olef_16 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3-6H,1H2,2H3
 C7H9r_R5_3 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h3H,1-2,4-5H2
 C7H9r_R5_8 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h4-5H,1,3H2,2H3
 C7H9r_R5_4 !! InChI=1S/C7H9/c1-6-4-3-5-7(6)2/h4H,1-3,5H2
 Ccy(C*CCCJC*C) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,5-6H,4H2,1H3
 CJcy(C*CC*CCC) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,5H,1,4,6H2
 CJcy(C*CCC*CC) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,6H,1,4-5H2
 C*cy(CCC*CCJC) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-4H,1,5-6H2
 CJcy(CC*CC*CC) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-5,7H,1,6H2
 Ccy(CJCC*CC*C) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-5H,6H2,1H3
 Ccy(CCJC*CC*C) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-7H,1H3
 C7H9r_Olef !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3,5-6H,1-2,4H2
 C*cy(CC*CCCJC) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3-5H,1-2,6H2
 Ccy(C*CCJCC*C) !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3-6H,2H2,1H3
 C7H9r_Olef_1 !! InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3-7H,1-2H2
 C*CCJ*CCC*C!! InChI=1S/C7H9/c1-3-5-7-6-4-2/h3-4,7H,1-2,5H2
 C*CCcy(C*CCC*C) !! InChI=1S/C8H10/c1-2-5-8-6-3-4-7-8/h2-3,6-7H,1,4-5H2
 C*CCcyCC*CC*C !! InChI=1S/C8H10/c1-2-5-8-6-3-4-7-8/h2-4,6-8H,1,5H2
 C*CCcy(C*CC*CC) !! InChI=1S/C8H10/c1-2-5-8-6-3-4-7-8/h2-4,6H,1,5,7H2
 C*CCCJCCC*C!! InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3-4,7H,1-2,5-6,8H2
 C*CC(CJ)CCC*C !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5,8H,1-3,6-7H2
 C*CC(C)CCJC*C !! InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-6,8H,1-2,7H2,3H3
 C*CCCCJCCC !! InChI=1S/C8H15/c1-3-5-7-8-6-4-2/h3,8H,1,4-7H2,2H3
 C*CCJCC(C)CC !! InChI=1S/C8H15/c1-4-6-7-8(3)5-2/h4,6,8H,1,5,7H2,2-3H3
 C*CCCC(CJ)CC !! InChI=1S/C8H15/c1-4-6-7-8(3)5-2/h4,8H,1,3,5-7H2,2H3
 C#CCcyCC*CC*C !! InChI=1S/C8H8/c1-2-5-8-6-3-4-7-8/h1,3-4,6-8H,5H2
 C*CC*cyCC*CC*C !! InChI=1S/C8H8/c1-2-5-8-6-3-4-7-8/h2-7H,1H2
 C*C*CcyCC*CC*C !! InChI=1S/C8H8/c1-2-5-8-6-3-4-7-8/h3-8H,1H2
 C6H5C2H3 !! InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2
 C*CC*cyCCJCC*C !! InChI=1S/C8H9/c1-2-5-8-6-3-4-7-8/h2-3,5-7H,1,4H2
 C*CCcyCJC*CC*C !! InChI=1S/C8H9/c1-2-5-8-6-3-4-7-8/h2-4,6-7H,1,5H2
 C*CC*cyCCJC*CC !! InChI=1S/C8H9/c1-2-5-8-6-3-4-7-8/h2-6H,1,7H2

C*CCJcyCC*CC*C !! InChI=1S/C8H9/c1-2-5-8-6-3-4-7-8/h2-8H,1H2
bicyclicC8H9 !! InChI=1S/C8H9/c1-2-6-7-4-3-5-8(6)7/h2-8H,1H2
C*CcyCC*CC*CCJ !! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h2-8H,1H2
C*CCCCJCCC*C !! InChI=1S/C9H15/c1-3-5-7-9-8-6-4-2/h3-4,9H,1-2,5-8H2
C*CCCC(CJ)CC*C !! InChI=1S/C9H15/c1-4-6-8-9(3)7-5-2/h4-5,9H,1-3,6-8H2
C*CCJCC(C)CC*C !! InChI=1S/C9H15/c1-4-6-8-9(3)7-5-2/h4-6,9H,1-2,7-8H2,3H3
C9H8 !! InChI=1S/C9H8/c1-2-5-9-7-3-6-8(9)4-1/h1-6H,7H2
Indene3AH !! InChI=1S/C9H8/c1-2-5-9-7-3-6-8(9)4-1/h1-8H
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
C7H7_3
C7H7_4
cC7H7
C7H7_6
C7H7_7
C7H7_8
C7H7_10
C7H7_11
C#Ccy(C*CC*CC)
C7H7_13

C7H7_14
C7H7_15
fulvenallene
cy (CJCCC*CCC) !! InChI=1S/C7H11/c1-2-4-6-7-5-3-1/h1-2, 7H, 3-6H2
cy (C*CCC*CCC) !! InChI=1S/C7H10/c1-2-4-6-7-5-3-1/h1-2, 5, 7H, 3-4, 6H2
C6H5C*CC*C !! InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h2-9H, 1H2
C6H5CJCC*C !! InChI=1S/C10H11/c1-2-3-7-10-8-5-4-6-9-10/h2, 4-9H, 1, 3H2
C6H5CCJC*C !! InChI=1S/C10H11/c1-2-3-7-10-8-5-4-6-9-10/h2-6, 8-9H, 1, 7H2
C6H5CJC*CC !! InChI=1S/C10H11/c1-2-3-7-10-8-5-4-6-9-10/h2-9H, 1H3
C6H5C*CCCJ !! InChI=1S/C10H11/c1-2-3-7-10-8-5-4-6-9-10/h3-9H, 1-2H2
C6H5CCC*C !! InChI=1S/C10H12/c1-2-3-7-10-8-5-4-6-9-10/h2, 4-6, 8-9H, 1, 3, 7H2
C6H5CC*CC !! InChI=1S/C10H12/c1-2-3-7-10-8-5-4-6-9-10/h2-6, 8-9H, 7H2, 1H3
C6H5C*CCC !! InChI=1S/C10H12/c1-2-3-7-10-8-5-4-6-9-10/h3-9H, 2H2, 1H3
C6H5CCCJC !! InChI=1S/C10H13/c1-2-3-7-10-8-5-4-6-9-10/h2, 4-6, 8-9H, 3, 7H2, 1H3
C6H5CCJCC !! InChI=1S/C10H13/c1-2-3-7-10-8-5-4-6-9-10/h3-6, 8-9H, 2, 7H2, 1H3
C6H5CCCCJ !! InChI=1S/C10H13/c1-2-3-7-10-8-5-4-6-9-10/h4-6, 8-9H, 1-3, 7H2
C6H5CJCCC !! InChI=1S/C10H13/c1-2-3-7-10-8-5-4-6-9-10/h4-9H, 2-3H2, 1H3
C6H5CC !! InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h3-7H, 2H2, 1H3
C6H5C2H3 !! InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H, 1H2
C6H5CJC !! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h2-7H, 1H3
C6H5CCJ !! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h3-7H, 1-2H2
C6H5CC*C !! InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-5, 7-8H, 1, 6H2
C6H5C*CC !! InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-8H, 1H3
C6H5CCJC !! InChI=1S/C9H11/c1-2-6-9-7-4-3-5-8-9/h2-5, 7-8H, 6H2, 1H3
C6H5CCCJ !! InChI=1S/C9H11/c1-2-6-9-7-4-3-5-8-9/h3-5, 7-8H, 1-2, 6H2
C6H5CJCC !! InChI=1S/C9H11/c1-2-6-9-7-4-3-5-8-9/h3-8H, 2H2, 1H3
C6H5CCC !! InChI=1S/C9H12/c1-2-6-9-7-4-3-5-8-9/h3-5, 7-8H, 2, 6H2, 1H3
C6H5CJC*C !! InChI=1S/C9H9/c1-2-6-9-7-4-3-5-8-9/h2-8H, 1H2
C6H5CJC*C-cy !! InChI=1S/C9H9/c1-2-5-9-7-3-6-8 (9) 4-1/h1-6, 9H, 7H2
C6H5CJC*CC-cy !! InChI=1S/C10H11/c1-8-6-7-9-4-2-3-5-10 (8) 9/h2-8, 10H, 1H3
C6H5CCJC*C-cy !! InChI=1S/C10H11/c1-2-6-10-8-4-3-7-9 (10) 5-1/h1-6, 9H, 7-8H2
M1H1Indene !! InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10 (8) 9/h2-8H, 1H3
C6H5CCCCJ-cy !! InChI=1S/C10H13/c1-2-6-10-8-4-3-7-9 (10) 5-1/h1-2, 5-6, 9H, 3-4, 7-8H2
C6H5CCCJC-cy !! InChI=1S/C10H13/c1-8-6-7-9-4-2-3-5-10 (8) 9/h2-5, 8, 10H, 6-7H2, 1H3
C6H5CCCCJ-cy !! InChI=1S/C9H11/c1-2-5-9-7-3-6-8 (9) 4-1/h1-2, 4-5, 8H, 3, 6-7H2
C*CCCJCC*C !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-4, 7H, 1-2, 5-6H2
C*CC*CCCJC !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-5, 7H, 1, 6H2, 2H3
CC*CC*CCCJ !! InChI=1S/C7H11/c1-3-5-7-6-4-2/h4-7H, 1, 3H2, 2H3
C*CC*CC*CC !! InChI=1S/C7H10/c1-3-5-7-6-4-2/h3-7H, 1H2, 2H3
C*CC*CCC*C !! InChI=1S/C7H10/c1-3-5-7-6-4-2/h3-5, 7H, 1-2, 6H2
O*cy (CC*CCC) !! InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1, 3H, 2, 4H2
JOOcy (CC*CCC) !! InChI=1S/C5H7O2/c6-7-5-3-1-2-4-5/h1, 3, 5H, 2, 4H2
JOcy (CC*CCC) !! InChI=1S/C5H7O/c6-5-3-1-2-4-5/h1, 3, 5H, 2, 4H2
HOOCy (CC*CCC) !! InChI=1S/C5H8O2/c6-7-5-3-1-2-4-5/h1, 3, 5-6H, 2, 4H2
O*cy (CC*CC*CC) !! InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-4H, 5H2
O*cy (CC*CCC*C) !! InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h2-5H, 1H2
JOcy (CC*CC*CC) !! InChI=1S/C6H7O/c7-6-4-2-1-3-5-6/h1-4, 6H, 5H2
JOcy (CC*CCC*C) !! InChI=1S/C6H7O/c7-6-4-2-1-3-5-6/h2-6H, 1H2

HOOCy (CC*CCC*C) !! InChI=1S/C6H8O2/c7-8-6-4-2-1-3-5-6/h2-7H,1H2
 HOOCy (CC*CC*CC) !! InChI=1S/C6H8O2/c7-8-6-4-2-1-3-5-6/h1-4,6-7H,5H2
 HOcy (CCJCC*CC) !! InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h1-2,5-7H,3-4H2
 JOcy (CCPC*CC) !! InChI=1S/C5H7O3/c6-4-2-1-3-5(4)8-7/h1,3-5,7H,2H2
 O*CC*CCCC*O !! InChI=1S/C6H8O2/c7-5-3-1-2-4-6-8/h1,3,5-6H,2,4H2
 JOOCyCCOHC*CCC !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h1,3,5-7H,2,4H2
 HOcy (CCJC*CCC) !! InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h1-2,4,6-7H,3,5H2
 O*CC*CCCCJOOH !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6-9-8/h1,3,5-6,8H,2,4H2
 O*CCCC*O !! InChI=1S/C5H8O2/c6-4-2-1-3-5-7/h4-5H,1-3H2
 JOcy (CCPCCC) !! InChI=1S/C5H9O3/c6-4-2-1-3-5(4)8-7/h4-5,7H,1-3H2
 HOcyCCJC*CC !! InChI=1S/C5H7O/c6-5-3-1-2-4-5/h1-3,5-6H,4H2
 O*CCCCJOOH !! InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h4-5,7H,1-3H2
 JOcy (CCPCC*CC) !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h1-2,5-6,8H,3-4H2
 JOOCyCCOHC*CC !! InChI=1S/C5H7O3/c6-4-2-1-3-5(4)8-7/h1-2,4-6H,3H2
 O*CCC*CCCJOOH !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6-9-8/h1-2,5-6,8H,3-4H2
 HOcy (CCJCCCC) !! InChI=1S/C6H11O/c7-6-4-2-1-3-5-6/h4,6-7H,1-3,5H2
 O*CCCCCJOOH !! InChI=1S/C6H11O3/c7-5-3-1-2-4-6-9-8/h5-6,8H,1-4H2
 O*CCCC*CCJOOH !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6-9-8/h2,4-6,8H,1,3H2
 JOOCyCCOHC*CC !! InChI=1S/C5H9O3/c6-4-2-1-3-5(4)8-7/h4-6H,1-3H2
 JOOCyCC*CCOHC !! InChI=1S/C5H7O3/c6-4-1-2-5(3-4)8-7/h1-2,4-6H,3H2
 O*CC*CCCJOOH !! InChI=1S/C5H7O3/c6-4-2-1-3-5-8-7/h1-2,4-5,7H,3H2
 JOcyCCPCCCC !! InChI=1S/C6H11O3/c7-5-3-1-2-4-6(5)9-8/h5-6,8H,1-4H2
 O*CCPC*CCCJ !! InChI=1S/C6H9O3/c1-2-3-4-6(5-7)9-8/h3-6,8H,1-2H2
 JOOCyCC*CCOHC*CC !! InChI=1S/C6H9O3/c7-5-1-3-6(9-8)4-2-5/h1,3,5-7H,2,4H2
 O*CCC*CCJOOH !! InChI=1S/C5H7O3/c6-4-2-1-3-5-8-7/h1,3-5,7H,2H2
 O*CCPCCCJ !! InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h4-5,7H,1-3H2
 JOOCyCCOHC*CC*CC !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h2,4-7H,1,3H2
 JOOCyCCOHC*CC*CC !! InChI=1S/C6H11O3/c7-5-3-1-2-4-6(5)9-8/h5-7H,1-4H2
 JOcyCCPCCC*CC !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h1,3,5-6,8H,2,4H2
 JOcyCCPCC*CC !! InChI=1S/C5H7O3/c6-4-2-1-3-5(4)8-7/h1-2,4-5,7H,3H2
 JOOCyCCOHC*CC*CC !! InChI=1S/C5H7O3/c6-4-2-1-3-5(4)8-7/h1,3-6H,2H2
 O*CCCC*O !! InChI=1S/C6H10O2/c7-5-3-1-2-4-6-8/h5-6H,1-4H2
 JOcyCCPC*CCC !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h2,4-6,8H,1,3H2
 HOcyCCJCCC !! InChI=1S/C5H9O/c6-5-3-1-2-4-5/h3,5-6H,1-2,4H2
 O*CCC*CCC*O !! InChI=1S/C6H8O2/c7-5-3-1-2-4-6-8/h1-2,5-6H,3-4H2
 O*CCPCCCCJ !! InChI=1S/C6H11O3/c1-2-3-4-6(5-7)9-8/h5-6,8H,1-4H2
 JOOCyCCOHC*CC*CC !! InChI=1S/C6H9O3/c7-5-3-1-2-4-6(5)9-8/h1-2,5-7H,3-4H2
 HOcyCCJCCC*CC !! InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h2,4-7H,1,3H2
 O*CCPCJC*CC !! InChI=1S/C5H7O3/c1-2-3-5(4-6)8-7/h2-5,7H,1H2
 O*CCPCCJC*CC !! InChI=1S/C6H9O3/c1-2-3-4-6(5-7)9-8/h2-3,5-6,8H,1,4H2
 HOcyCCJCC*CC !! InChI=1S/C5H7O/c6-5-3-1-2-4-5/h1,3-6H,2H2
 C6H5CH2OOH
 C6H5CH2O
 C6H5CHO
 C6H5C2H2
 C6H5CO
 C6H5CPC
 C6H5C(OJ)C
 C*CC*CCJC*O !! InChI=1S/C6H7O/c1-2-3-4-5-6-7/h2-6H,1H2
 CJCCCC*O !! InChI=1S/C5H9O/c1-2-3-4-5-6/h5H,1-4H2

CCJCCC*O !! InChI=1S/C5H9O/c1-2-3-4-5-6/h2, 5H, 3-4H2, 1H3
 C*CCJCCy (COC) !! InChI=1S/C6H9O/c1-2-3-4-6-5-7-6/h2-3, 6H, 1, 4-5H2
 CJCCCcy (COC) !! InChI=1S/C6H11O/c1-2-3-4-6-5-7-6/h6H, 1-5H2
 HOCCJC*CCC*O !! InChI=1S/C6H9O2/c7-5-3-1-2-4-6-8/h1-3, 6-7H, 4-5H2
 CJC (OH) CCcy (COC) !! InChI=1S/C6H11O2/c1-5 (7) 2-3-6-4-8-6/h5-7H, 1-4H2
 CJC (OH) C*CCC*O !! InChI=1S/C6H9O2/c1-6 (8) 4-2-3-5-7/h2, 4-6, 8H, 1, 3H2
 HOCCJCCcy (COC) !! InChI=1S/C6H11O2/c7-4-2-1-3-6-5-8-6/h2, 6-7H, 1, 3-5H2
 CJC (OH) CCC*O !! InChI=1S/C5H9O2/c1-5 (7) 3-2-4-6/h4-5, 7H, 1-3H2
 CCJCCcy (COC) !! InChI=1S/C6H11O/c1-2-3-4-6-5-7-6/h2, 6H, 3-5H2, 1H3
 C*CCCJCC*O !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2, 4, 6H, 1, 3, 5H2
 CC*CCJCC*O !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-4, 6H, 5H2, 1H3
 C*CCJC (OH) CC*O !! InChI=1S/C6H9O2/c1-2-3-6 (8) 4-5-7/h2-3, 5-6, 8H, 1, 4H2
 C*CC*CCOH !! InChI=1S/C5H8O/c1-2-3-4-5-6/h2-4, 6H, 1, 5H2
 C*CC (OH) C*C !! InChI=1S/C5H8O/c1-3-5 (6) 4-2/h3-6H, 1-2H2
 CJCC*CCC*O !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h3-4, 6H, 1-2, 5H2
 C*CCJCCC*O !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-3, 6H, 1, 4-5H2
 HOCCJCCC*O !! InChI=1S/C5H9O2/c6-4-2-1-3-5-7/h2, 5-6H, 1, 3-4H2
 C*CC (OH) CJCC*O !! InChI=1S/C6H9O2/c1-2-6 (8) 4-3-5-7/h2, 4-6, 8H, 1, 3H2
 C*CCCCOJ !! InChI=1S/C4H7O2/c1-2-3-4-6-5/h2H, 1, 3-4H2
 JOOcy (CCCC) !! InChI=1S/C5H9O2/c6-7-5-3-1-2-4-5/h5H, 1-4H2
 cy (CC*CcyCOCC) !! InChI=1S/C6H8O/c1-2-5-4-7-6 (5) 3-1/h1, 3, 5-6H, 2, 4H2
 HOOcy (CC*CC*C) !! InChI=1S/C5H6O2/c6-7-5-3-1-2-4-5/h1-6H
 C*CC*CC*CJ !! InChI=1S/C6H7/c1-3-5-6-4-2/h1, 3-6H, 2H2
 JOOCcy (CC*CCC) !! InChI=1S/C6H9O2/c7-8-5-6-3-1-2-4-6/h1, 3, 6H, 2, 4-5H2
 HOOcy (CC*CCCC) !! InChI=1S/C6H10O2/c7-8-6-4-2-1-3-5-6/h2, 4, 6-7H, 1, 3, 5H2
 CJCCC*CC*O !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h4-6H, 1-3H2
 JOcy (CC*CCCC) !! InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h2, 4, 6H, 1, 3, 5H2
 JOcy (CCC*CCC) !! InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h1-2, 6H, 3-5H2
 HOOcy (CCC*CCC) !! InChI=1S/C6H10O2/c7-8-6-4-2-1-3-5-6/h1-2, 6-7H, 3-5H2
 HOCJcyCCC*CC !! InChI=1S/C6H9O/c7-5-6-3-1-2-4-6/h1-2, 5-7H, 3-4H2
 HOCOOJcyCC*CCC !! InChI=1S/C6H9O3/c7-6 (9-8) 5-3-1-2-4-5/h1, 3, 5-7H, 2, 4H2
 O*CcyCC*CCC !! InChI=1S/C6H8O/c7-5-6-3-1-2-4-6/h1, 3, 5-6H, 2, 4H2
 HOCJcyCC*CCC !! InChI=1S/C6H9O/c7-5-6-3-1-2-4-6/h1, 3, 5-7H, 2, 4H2
 HOC*cyCC*CCC !! InChI=1S/C6H8O/c7-5-6-3-1-2-4-6/h1, 3, 5, 7H, 2, 4H2
 C*CCJCC*COH !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-3, 5-7H, 1, 4H2
 CJCC*CC*COH !! InChI=1S/C6H9O/c1-2-3-4-5-6-7/h3-7H, 1-2H2
 HOCOOJcyCCC*CC !! InChI=1S/C6H9O3/c7-6 (9-8) 5-3-1-2-4-5/h1-2, 5-7H, 3-4H2
 O*CcyCCC*CC !! InChI=1S/C6H8O/c7-5-6-3-1-2-4-6/h1-2, 5-6H, 3-4H2
 C*CCC (C) CJ !! InChI=1S/C6H11/c1-4-5-6 (2) 3/h4, 6H, 1-2, 5H2, 3H3
 Ccy (CJCCCC) !! InChI=1S/C6H11/c1-6-4-2-3-5-6/h2-5H2, 1H3
 Ccy (C*CCCC) !! InChI=1S/C6H10/c1-6-4-2-3-5-6/h4H, 2-3, 5H2, 1H3
 JOOcy (CCC*CC) !! InChI=1S/C5H7O2/c6-7-5-3-1-2-4-5/h1-2, 5H, 3-4H2
 C*CC (CJ) C !! InChI=1S/C5H9/c1-4-5 (2) 3/h4-5H, 1-2H2, 3H3
 C*CCJCCC !! InChI=1S/C5H9/c1-3-5-4-2/h1, 4-5H2, 2H3
 CJ*CCCC !! InChI=1S/C5H9/c1-3-5-4-2/h1, 3H, 4-5H2, 2H3
 HOcy (CCC*CCC) !! InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-2, 6-7H, 3-5H2
 HOcyCCCC (OOJ) CC !! InChI=1S/C6H11O3/c7-5-1-3-6 (9-8) 4-2-5/h5-7H, 1-4H2
 HOcy (CCCCJCC) !! InChI=1S/C6H11O/c7-6-4-2-1-3-5-6/h1, 6-7H, 2-5H2
 C*CC (OH) CCC*O !! InChI=1S/C6H10O2/c1-2-6 (8) 4-3-5-7/h2, 5-6, 8H, 1, 3-4H2
 CC*CCOOH !! InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3, 5H, 4H2, 1H3
 HOcyCCJCCPCC !! InChI=1S/C6H11O3/c7-5-1-3-6 (9-8) 4-2-5/h1, 5-8H, 2-4H2

C*CC(C)OOH !! InChI=1S/C4H8O2/c1-3-4(2)6-5/h3-5H,1H2,2H3
 CC*CCOJ !! InChI=1S/C4H7O/c1-2-3-4-5/h2-3H,4H2,1H3
 CH2CHOO !! InChI=1S/C2H3O2/c1-2-4-3/h2H,1H2
 END

THERMO ALL

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 0.00000000E+00 3
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 0.26219035E+05 4
 H2 TPIS78H 2 0 0 0G 200.000 6000.00 1000.00
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 0.00000000E+00 4
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 4.48613328E+03 4
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 0.02387202E-07-0.08431442E-11 5.00213000E+04 0.13588605E+01
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 0.29084817E+05 4
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 16 2
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 0.47328105E+05 4
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 05 3
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 5.08749163E+03 4
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 14 2
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 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 1 C 1 O 2 0 G 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 4O 3 OG 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 OG 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 9/ 1/12 C 1H 30 3 OG 300.000 5000.000
 997.000 21
 2.22488435E+00 1.70328727E-02-6.24631476E-06 8.37499249E-10-3.22096209E-14 2
 6.04759781E+03 2.33052848E+01 1.92120102E+00 3.09717915E-02-3.38215757E-05 3
 1.93739647E-08-4.63932897E-12 4.86086899E+03 2.02247107E+01
 4
 HOCH2O 2/16/99 THERMC 1H 30 2 OG 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
 HOCH2O2H 4/ 9/98 THERMC 1H 40 3 OG 300.000 5000.000
 1422.000 31
 1.16303827E+01 7.15133688E-03-2.39035030E-06 3.65772791E-10-2.10199524E-14 2
 -4.31079242E+04-3.24276725E+01 1.85716693E+00 3.23153132E-02-2.69928902E-05 3
 1.11694484E-08-1.81284103E-12-4.00314471E+04 1.90917729E+01
 4
 HOCH2O2 4/ 9/98 THERMC 1H 30 3 OG 300.000 5000.000
 1412.000 21
 9.04545938E+00 7.15223373E-03-2.37005676E-06 3.60083481E-10-2.05750228E-14 2
 -2.49414886E+04-1.74210530E+01 2.85441621E+00 2.33663535E-02-1.88115990E-05 3
 7.96709515E-09-1.36346618E-12-2.29866196E+04 1.51730565E+01
 4
 OCH2O2H 4/ 9/98 THERMC 1H 30 3 OG 300.000 5000.000
 1420.000 21
 1.15398246E+01 5.34291432E-03-1.81878917E-06 2.81968625E-10-1.63584348E-14 2
 -1.68237489E+04-3.20700633E+01 1.93823075E+00 3.01465730E-02-2.61053152E-05 3
 1.09463562E-08-1.78312692E-12-1.38166625E+04 1.85042002E+01
 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 300.00 5000.00 1000.00
 1
 4.80390863E+00 9.95844638E-03-3.85301026E-06 6.84740497E-10-4.58402955E-
 14 2
 -7.47135460E+02 1.45281400E+00 3.62497097E+00 3.59397933E-03 2.26538097E-
 05 3
 -2.95391947E-08 1.11977570E-11 7.93040410E+01 9.96382194E+00
 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
 1
 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 5O 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 6O 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 5O 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 5O 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
 CH3CHO2H 9/ 1/12 C 2H 5O 2 0G 300.000 5000.000
 1386.000 31
 9.94166406E+00 1.14384962E-02-3.92847407E-06 6.11402143E-10-3.55267132E-
 14 2
 -2.02545876E+03-2.22163407E+01 4.16440687E+00 2.38795950E-02-1.46887446E-
 05 3
 5.18066666E-09-8.37968487E-13 1.87348817E+02 9.35429162E+00
 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
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 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-
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 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 ATCT AC 3 H 6 O 1 0 G 200.000 6000.00 1000.00
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 7.29796974E+00 1.75656913E-02-6.31678065E-06 1.02025553E-09-6.10903592E-
 14 2
 -2.95368927E+04-1.27591704E+01 5.55638920E+00-2.83863547E-03 7.05722951E-
 05 3
 -8.78130984E-08 3.40290951E-11-2.78325393E+04 2.31960221E+00-
 2.58360384E+04 4
 CH3COCH2 A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00
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 14 2
 -7.48672286E+03-1.14792587E+01 4.70187196E+00 5.51653762E-03 4.27505858E-
 05 3
 -5.94680816E-08 2.40685378E-11-5.92845491E+03 7.12932590E+00-
 4.00985747E+03 4
 CH3COCH2O2 2/14/95 C 3H 5O 3 OG 300.000 5000.000 1379.00
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 14 2
 -2.34798669E+04-3.27155799E+01 5.95535468E+00 2.70255205E-02-1.37385031E-
 05 3
 3.53735851E-09-4.03922557E-13-2.06679464E+04 5.21436049E+00
 4
 CH3COCH2O2H 2/14/95 C 3H 6O 3 OG 300.000 5000.000 1381.00
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 14 2
 -4.27564444E+04-4.77383784E+01 4.94789761E+00 3.60474432E-02-2.21719933E-
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 6.98296874E-09-9.21269260E-13-3.88687178E+04 8.49926130E+00
 4
 CH3COCH2O 4/ 3/ 0 THERMC 3H 5O 2 OG 300.000 5000.000
 1370.000 21
 1.14637586E+01 1.32124342E-02-4.56580495E-06 7.13897538E-10-4.16281047E-
 14 2
 -2.23833017E+04-3.15127868E+01 3.72927689E+00 2.63943697E-02-1.09796486E-
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 4
 C2H3OCH2 H 5 C 3 O 1 G 298.0 6000.0
 1000.0 1
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 C2H3CHO H 4 C 3 O 1 G 298.0 6000.0
 1000.0 1
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 14 2
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 6.09330392E-08-2.17017624E-11-8.41778158E+03 2.84760680E+01
 4
 C2H3CO KPS12 C 3H 3O 1 OG 300.000 5000.000
 1395.000 01
 8.86032735E+00 8.48985205E-03-2.90350080E-06 4.50763986E-10-2.61524281E-
 14 2
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 05 3
 7.29174972E-09-1.16083226E-12 1.02020654E+04 1.78705872E+01
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 C3H5O H 5 C 3 O 1 G 298.0 6000.0
 1000.0 1
 9.34720957E+00 1.30735257E-02-4.58398309E-06 7.26633413E-10-4.29140495E-
 14 2
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 05 3
 5.84958068E-08-2.04960267E-11 1.12279936E+04 3.09764754E+01
 4
 C2H5CHO T05/10C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
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 2.22688471E+04 4
 C2H5CO A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00
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 05 3
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 3.94851891E+03 4
 CH2CH2CHO H 5 C 3 O 1 G 298.0 6000.0
 1000.0 1
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 14 2
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 4.00355717E-08-1.52720345E-11 1.80133296E+03 1.64536197E+01
 4
 CH3CHCHO 8/10/ 4 THERMC 3H 5O 1 OG 300.000 5000.000
 1253.000 21
 8.27772090E+00 1.95687188E-02-8.47575089E-06 1.53249728E-09-9.86441542E-
 14 2
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 05 3

5.09554570E-09-7.28789092E-13-3.51122739E+03 4.04496677E+01
 4
 CH3OCH3 1/20/11 C 2H 60 1 0G 300.000 5000.000
 1367.000 21
 7.36358679E+00 1.38910153E-02-4.74083257E-06 7.34874498E-10-4.25867578E-14 2
 -2.61148074E+04-1.61332876E+01 2.41860337E+00 1.87279640E-02-1.40894592E-06 3
 -4.28367822E-09 1.36818123E-12-2.36771735E+04 1.28877967E+01
 4
 CH3OCH2 1/20/11 C 2H 50 1 0G 300.000 5000.000
 1389.000 21
 6.73134670E+00 1.18022530E-02-4.00104434E-06 6.17227325E-10-3.56435023E-14 2
 -3.34933412E+03-9.40782513E+00 2.19172957E+00 1.90390966E-02-6.81450700E-06 3
 8.63577609E-11 3.23902492E-13-1.38948253E+03 1.62440756E+01
 4
 CH3OCH2O2 1/20/11 C 2H 50 3 0G 300.000 5000.000
 1399.000 31
 1.22024149E+01 1.19225104E-02-4.06624713E-06 6.30079576E-10-3.65065312E-14 2
 -2.40327175E+04-3.38665462E+01 1.72101041E+00 3.78155492E-02-2.89668870E-05 3
 1.16796117E-08-1.93234479E-12-2.05308597E+04 2.19296296E+01
 4
 CH2OCH2O2H 1/20/11 C 2H 50 3 0G 300.000 5000.000
 1419.000 41
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 -1.96611854E+04-4.85172618E+01 9.08332173E-01 4.47997444E-02-3.69441578E-05 3
 1.48366604E-08-2.32279459E-12-1.50992319E+04 2.66419885E+01
 4
 CH3OCH2O2H 1/20/11 C 2H 60 3 0G 300.000 5000.000
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 1.46617126E+01 1.20544674E-02-4.13604704E-06 6.43721637E-10-3.74188832E-14 2
 -4.18896186E+04-4.81293252E+01 7.37369081E-01 4.67410003E-02-3.73051936E-05 3
 1.50735309E-08-2.43781978E-12-3.73260287E+04 2.57932851E+01
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 CH3OCH2O 2/ 9/96 THERMC 2H 50 2 0G 300.000 5000.000
 2012.000 21
 8.60261845E+00 1.35772195E-02-4.84661602E-06 7.77766193E-10-4.62633624E-14 2
 -2.13762444E+04-1.75775023E+01 3.25889339E+00 2.22146359E-02-7.78556340E-06 3
 -2.41484158E-10 4.51914496E-13-1.92377212E+04 1.23680069E+01
 4
 O2CH2OCH2O2H 1/20/11 C 2H 50 5 0G 300.000 5000.000
 1411.000 51
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 -3.98679641E+04-6.72721405E+01-1.22579809E-01 6.64376755E-02-6.55340609E-05 3
 3.13441786E-08-5.79042960E-12-3.41530358E+04 3.49112501E+01
 4

HO2CH2OCHO 1/20/11 C 2H 4O 4 OG 300.000 5000.000
 1428.000 41
 1.78528337E+01 7.54042388E-03-2.74895624E-06 4.45343367E-10-2.66154007E-
 14 2
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 05 3
 1.24225089E-08-1.50813145E-12-5.82730214E+04 2.81992694E+01
 4
 OCH2OCHO 1/20/11 C 2H 3O 3 OG 300.000 5000.000
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 1.24378042E+01 7.82259106E-03-2.82874305E-06 4.55808935E-10-2.71391601E-
 14 2
 -4.44526361E+04-3.85337353E+01 3.92797655E+00 1.85731220E-02-4.14656828E-
 07 3
 -6.94060480E-09 2.32311215E-12-4.07070844E+04 1.02048630E+01
 4
 HOCH2OCO 8/31/99 THERMC 2H 3O 3 OG 300.000 5000.000
 1603.000 31
 1.13737391E+01 8.17663898E-03-2.92034021E-06 4.66695616E-10-2.76276823E-
 14 2
 -4.65575743E+04-2.86035265E+01 6.08180801E+00 1.28768359E-02 2.04419418E-
 06 3
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 4
 CH3OCHO T 6/08C 2 H 4 O 2 0 G 200.000 6000.00 1000.00
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 14 2
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 05 3
 -8.29932227E-08 3.13522917E-11-4.55713267E+04 7.50341113E-01-
 4.37330508E+04 4
 CH3OCO 5/ 8/ 3 THERMC 2H 3O 2 OG 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 3O 2 OG 300.000 5000.000
 1442.000 21
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 06 3
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 4
 HE G 5/97HE 1 0 0 0 G 200.000 6000.00 1000.00
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 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 2
 -7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00
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 0.00000000E+00 4
 C3H8 G 2/00C 3 H 8 0 0 G 200.000 6000.00 1000.00
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6.66919760E+00 2.06108751E-02-7.36512349E-06 1.18434262E-09-7.06914630E-
14 2
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05 3
-9.20060565E-08 3.64618453E-11-1.43810883E+04 5.61004451E+00-
1.25900384E+04 4
NC3H7 A 5/05C 3 H 7 0 0 G 200.000 6000.00 1000.00
1
6.49636579E+00 1.77337992E-02-6.24898046E-06 9.95389495E-10-5.90199770E-
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05 3
-6.99343598E-08 2.81819493E-11 1.04074558E+04 8.39534919E+00
1.21859256E+04 4
IC3H7 A 5/05C 3 H 7 0 0 G 200.000 6000.00 1000.00
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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
C3H6 G 2/00C 3 H 6 0 0 G 200.000 6000.00 1000.00
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14 2
-7.41715057E+02-8.43825992E+00 3.83464468E+00 3.29078952E-03 5.05228001E-
05 3
-6.66251176E-08 2.63707473E-11 7.88717123E+02 7.53408013E+00
2.40543339E+03 4
!C3H5-A PD5/98C 3H 5 0 0G 300.000 3000.00
1000.00 1
! 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
!-0.33355555E-07 0.15846571E-10 0.19245629E+05 0.17173214E+02
4
C3H5-T PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
1
0.54255528E+01 0.15511072E-01-0.56678350E-05 0.79224388E-09-0.16878034E-
13 2
0.27843027E+05-0.33527184E+01 0.17329209E+01 0.22394620E-01-0.51490611E-
05 3
-0.67596466E-08 0.38253211E-11 0.29040498E+05 0.16568878E+02
4
C3H5-S PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
1
0.53725281E+01 0.15780509E-01-0.59922850E-05 0.93089664E-09-0.36550966E-
13 2
0.29614760E+05-0.34186478E+01 0.91372931E+00 0.26432343E-01-0.11758950E-
04 3
-0.23035678E-08 0.27715488E-11 0.30916867E+05 0.19989269E+02
4
C3H4-A L 8/89C 3 H 4 0 0 G 200.000 6000.00 1000.00
1
0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-
13 2

0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-
 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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 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-
 13 2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-
 05 3
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 0.22302059E+05 4
 HCCCHCCH OC 5H 3 0 0G 200.000 5000.000 1000.00
 0 1
 0.10313636E+02 0.10278554E-01-0.37086568E-05 0.60568664E-09-0.36721455E-
 13 2
 0.65859508E+05-0.26380088E+02 0.10442368E+01 0.44574721E-01-0.50980758E-
 04 3
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 4
 C4H5C2H OC 6H 6 0 0G 200.000 5000.000 1100.00
 0 1
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 13 2
 0.35975470E+05-0.47671401E+02-0.23220260E+00 0.54092928E-01-0.36134322E-
 04 3
 0.69104632E-08 0.13734168E-11 0.39978520E+05 0.25932864E+02
 4
 FULVENE OC 6H 6 0 0G 200.000 5000.000 1000.00
 0 1
 0.11103525E+02 0.20600685E-01-0.75302224E-05 0.12388695E-08-0.75415976E-
 13 2
 0.20361843E+05-0.36665197E+02-0.71813191E+00 0.37934312E-01 0.11398837E-
 04 3
 -0.41333503E-07 0.18055927E-10 0.24223825E+05 0.27855714E+02
 4
 CHCCH2CH2CHCH2 C 6H 8 G 298.000 3000.000 1000.00
 1
 6.73656828E+00 3.59801214E-02-1.79442697E-05 4.36251971E-09-4.18063104E-
 13 2
 2.66969542E+04-5.89162957E+00 6.81481260E-01 5.74228263E-02-4.59418624E-
 05 3
 2.02499383E-08-3.69550697E-12 2.80468538E+04 2.40150759E+01
 4
 CH2CCHCH2CHCH2 C 6H 8 G 298.000 3000.000 1000.00
 1
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 13 2
 2.64952935E+04-1.70336741E+00 3.40906598E+00 3.94865090E-02-1.07919414E-
 05 3
 -8.29929939E-09 4.69973999E-12 2.74305565E+04 1.33764700E+01
 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-
 14 2
 3.95709594E+04-1.25848690E+01 1.35110873E+00 3.27411291E-02-4.73827407E-
 05 3

3.76310220E-08-1.18541128E-11 4.07679941E+04 1.52058598E+01
 4.22762135E+04 4
 C3H3O 1/31/13 C 3H 30 1 0G 300.000 5000.000
 1539.000 21
 1.53343473E+01 3.37165935E-03-1.47376680E-06 2.68145680E-10-1.73488725E-
 14 2
 2.24265932E+04-6.26451420E+01-1.26339760E+00 9.87046868E-03 3.01369100E-
 05 3
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 4
 C3H3O2H 1/31/13 C 3H 40 2 0G 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 20 1 0G 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
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 6.67324762E+00 5.57728845E-03-1.99180164E-06 3.20289156E-10-1.91216272E-
 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 0G 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 0G 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 0G 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
 -5.58295862E+03-4.28758364E+01 2.38465746E+00 4.42928555E-02-3.50977087E-05 3
 1.53695144E-08-2.81167824E-12-1.80979612E+03 1.69923285E+01
 4
 C3H6OOH2-2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1387.000 41
 1.28195023E+01 1.60998199E-02-5.51073827E-06 8.55673475E-10-4.96391225E-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
 1.81661664E+01 1.47644887E-02-4.74842743E-06 7.06972467E-10-3.98305587E-14 2
 -2.26256376E+04-5.93719393E+01 5.56933350E+00 4.68523421E-02-3.58917784E-05 3
 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-05 3
 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
 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-05 3
 1.77187019E-08-2.92768695E-12-2.02143526E+04 1.34150719E+01
 4
 NC3H7O T07/10C 3 H 7 O 1 0 G 200.000 6000.00 1000.00
 1

8.38041157E+00 1.95206120E-02-6.97374143E-06 1.12144919E-09-6.69467831E-
 14 2
 -8.48625211E+03-1.89916219E+01 4.21934640E+00 7.38556641E-03 6.02825529E-
 05 3
 -8.38680247E-08 3.39623435E-11-6.23491852E+03 8.08139850E+00-
 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-
 14 2
 -1.13388060E+04-3.60564653E+01 1.69886473E+00 3.63643211E-02-2.24587302E-
 05 3
 7.15111944E-09-9.33278403E-13-7.77098005E+03 1.69680075E+01
 4
 NC3H7O2H 9/ 1/12 C 3H 8O 2 OG 300.000 5000.000
 1394.000 41
 1.46883407E+01 1.60212483E-02-5.27531221E-06 7.98877253E-10-4.55711618E-
 14 2
 -2.90318646E+04-4.95529916E+01 9.13626931E-01 4.89566251E-02-3.51850148E-
 05 3
 1.30546796E-08-1.95621807E-12-2.43818102E+04 2.40611651E+01
 4
 NC3H7O2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1500.000 31
 1.36927178E+01 1.46801304E-02-4.79793976E-06 7.22768575E-10-4.10732852E-
 14 2
 -1.17561732E+04-4.32476343E+01 3.13948561E+00 3.66456006E-02-2.03703424E-
 05 3
 4.70670546E-09-1.99573208E-13-7.91997431E+03 1.42198984E+01
 4
 IC3H7O2H 9/ 1/12 C 3H 8O 2 OG 300.000 5000.000
 1393.000 41
 1.40855241E+01 1.75805904E-02-6.02432523E-06 9.36214739E-10-5.43465682E-
 14 2
 -3.06618857E+04-4.81005453E+01 1.47731961E+00 4.92440994E-02-3.79913951E-
 05 3
 1.61970607E-08-2.90125059E-12-2.63956602E+04 1.90105627E+01
 4
 IC3H7O2 9/ 1/12 C 3H 7O 2 OG 300.000 5000.000
 1395.000 31
 1.33991937E+01 1.58889581E-02-5.40791162E-06 8.36616758E-10-4.84119240E-
 14 2
 -1.34911944E+04-4.35329618E+01 3.42416052E+00 3.84321103E-02-2.50950244E-
 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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 6.80716906E+00 1.88824545E-02-6.79082475E-06 1.09713919E-09-6.57154952E-
 14 2
 -1.36547629E+04-1.35382154E+01 5.15283752E+00-1.86401716E-02 1.29980652E-
 04 3
 -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
C3KET12 7/19/ 0 THERMC 3H 60 3 0G 300.000 5000.000
1388.000 41
1.70756225E+01 1.31013491E-02-4.61949408E-06 7.31991329E-10-4.30788679E-
14 2
-4.17008637E+04-5.95778952E+01 1.10507238E+00 5.27396706E-02-4.31805774E-
05 3
1.81618292E-08-3.10535568E-12-3.63627536E+04 2.54111636E+01
4
C3KET13 7/19/ 0 THERMC 3H 60 3 0G 300.000 5000.000
1379.000 41
1.58927479E+01 1.40990923E-02-4.96118851E-06 7.84992198E-10-4.61488928E-
14 2
-3.93774829E+04-5.26049341E+01 3.55241022E+00 4.18720270E-02-2.94550370E-
05 3
1.09982900E-08-1.75045977E-12-3.48902671E+04 1.42082894E+01
4
C3KET21 7/19/ 0 THERMC 3H 60 3 0G 300.000 5000.000
1371.000 41
1.56377776E+01 1.44059342E-02-5.08808082E-06 8.07076119E-10-4.75295650E-
14 2
-4.30657975E+04-5.13105869E+01 4.55686367E+00 3.57076837E-02-1.94712054E-
05 3
4.70695431E-09-3.69753807E-13-3.86710975E+04 9.97761694E+00
4
C3H51-2,300H 8/26/3 THRMC 3H 70 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
C3H52-1,300H 8/26/3 THRMC 3H 70 4 0G 300.000 5000.000
1379.000 61
2.02817964E+01 1.48155431E-02-5.25503386E-06 8.35963453E-10-4.93308915E-
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 70 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
HOC3H6O2 9/ 1/12 C 3H 70 3 0G 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 0G 300.000 5000.000 1400.00
 41
 1.00219123E+01 9.56966300E-03-3.26221644E-06 5.05231706E-10-2.92593257E-
 14 2
 -1.42482738E+04-2.77829973E+01 1.48380119E+00 3.22203013E-02-2.70250033E-
 05 3
 1.20499164E-08-2.18365931E-12-1.15276540E+04 1.71552068E+01
 4
 AC3H5OOH GOLDSMITH C 3H 60 2 0G 298.0 6000.0
 1000.000 31
 1.20838649E+01 1.47946591E-02-5.13212591E-06 8.07504999E-10-4.74394983E-
 14 2
 -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 0G 300.000 5000.000
 1395.000 41
 1.47661443E+01 2.12235231E-02-7.09403390E-06 1.08423759E-09-6.22145708E-
 14 2
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 05 3
 1.32495013E-08-2.06619289E-12-8.87891782E+03 2.43857336E+01
 4
 C2H3OOH 4/18/ 8 THERMC 2H 40 2 0G 300.000 5000.000
 1397.000 21
 1.15749951E+01 8.09909174E-03-2.81808668E-06 4.42697954E-10-2.58998042E-
 14 2
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 1.14222854E-08-1.89488886E-12-5.49996692E+03 1.98354466E+01
 4
 C4H10 9/ 1/12 C 4H 10 0 0G 300.000 5000.000
 1389.000 31
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 14 2
 -2.18475689E+04-4.46643459E+01-4.02516492E-01 4.79826446E-02-2.65875714E-
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 7.07078402E-09-6.98493372E-13-1.68794837E+04 2.63198718E+01
 4
 PC4H9 9/ 1/12 C 4H 9 0 0G 300.000 5000.000
 1393.000 31
 1.18227273E+01 1.97584602E-02-6.73845199E-06 1.04383408E-09-6.04576130E-
 14 2
 3.50333683E+03-3.69846129E+01 3.50939027E-01 4.47616979E-02-2.76331489E-
 05 3
 9.10558432E-09-1.28318459E-12 7.74508072E+03 2.53924028E+01
 4
 SC4H9 9/ 1/12 C 4H 9 0 0G 300.000 5000.000
 1388.000 31
 1.11370287E+01 2.04038703E-02-6.97571297E-06 1.08244679E-09-6.27714790E-
 14 2
 1.95591491E+03-3.30856128E+01 6.23603962E-01 3.99289701E-02-1.89596886E-
 05 3
 3.45938210E-09-2.39235619E-14 6.17688777E+03 2.52737918E+01
 4

C4H8-1 T05/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
1
7.86795262E+00 2.24448843E-02-8.07705438E-06 1.30179988E-09-7.77958472E-
14 2
-4.23853340E+03-1.65662549E+01 5.13226136E+00 5.33862838E-03 6.02928960E-
05 3
-7.60364685E-08 2.87324693E-11-2.16718358E+03 3.82936810E+00-
3.72842176E+00 4
C4H8-2 T 5/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
1
7.89114667E+00 2.24970532E-02-8.12143779E-06 1.31273568E-09-7.84451632E-
14 2
-5.51643171E+03-1.76436027E+01 5.57278967E+00 3.76541017E-03 6.52226708E-
05 3
-8.30909522E-08 3.20311342E-11-3.60128327E+03 5.37796708E-01-
1.34523863E+03 4
C4H71-1 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
1
8.15646382E+00 1.90308835E-02-6.73262214E-06 1.07333098E-09-6.36886441E-
14 2
2.55826427E+04-1.61428872E+01 4.19857522E+00 1.19616999E-02 4.23864923E-
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
1
8.16688868E+00 1.95680375E-02-6.95694878E-06 1.11504166E-09-6.64079384E-
14 2
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05 3
-5.72714455E-08 2.36641011E-11 2.58014506E+04 9.11906641E+00
2.78022108E+04 4
!C4H71-3 T05/04C 4 H 7 0 0 G 200.000 6000.00
1000.00 1
! 8.08107449E+00 1.95526544E-02-6.93149115E-06 1.10889183E-09-
6.59584410E-14 2
! 1.22822959E+04-1.67137903E+01 4.54746808E+00 4.63771460E-03
6.61340221E-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 1
! 8.49073768E+00 1.91056974E-02-6.74370664E-06 1.07343267E-09-
6.36251837E-14 2
! 2.04659294E+04-1.74555814E+01 5.07355313E+00 5.27619329E-03
6.23441322E-05 3
!-8.54203458E-08 3.45890031E-11 2.24615054E+04 5.60318035E+00
2.46070249E+04 4
C4H72-2 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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7.26612168E+00 1.99858497E-02-7.12030976E-06 1.14276142E-09-6.81206632E-
14 2
2.31915554E+04-1.09941637E+01 7.61389036E+00-9.06922602E-03 8.28486476E-
05 3
-9.61203624E-08 3.59333528E-11 2.44971584E+04-5.90519467E+00
2.69231159E+04 4
C4H6 H6W/94C 4H 6 0 0G 300.000 3000.00 1000.00
1

0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-
 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
 4
 PC4H9O2H 9/ 1/12 C 4H 100 2 OG 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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 05 3
 1.63427400E-08-2.29549654E-12-2.71975592E+04 2.95249361E+01
 4
 PC4H9O2 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
 1663.000 41
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 14 2
 -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 OG 300.000 5000.000
 1395.000 51
 1.85276559E+01 1.96998004E-02-6.48703965E-06 9.82426308E-10-5.60434220E-
 14 2
 -3.51152892E+04-6.98322937E+01 4.05944553E-01 6.48970390E-02-4.98857846E-
 05 3
 2.00008685E-08-3.25194364E-12-2.91704448E+04 2.63739532E+01
 4
 SC4H9O2 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
 1408.000 41
 1.71094567E+01 1.90236957E-02-6.29508198E-06 9.55825976E-10-5.46024443E-
 14 2
 -1.76672012E+04-6.11399832E+01 2.68574393E+00 5.26273779E-02-3.56094836E-
 05 3
 1.22899616E-08-1.68623273E-12-1.27229421E+04 1.62316995E+01
 4
 PC4H9O 8/ 9/ 4 THERMC 4H 90 1 OG 300.000 5000.000
 1403.000 31
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 14 2
 -1.46178979E+04-5.25561919E+01-4.99964924E-01 5.37157310E-02-3.44426650E-
 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
 1679.000 31
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 14 2
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 C4H7O 4/ 3/ 0 THERMC 4H 70 1 OG 300.000 5000.000
 1395.000 21
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 C4H8O1-2 4/ 3/ 0 THERMC 4H 80 1 0G 300.000 5000.000
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 1.66679793E-08-2.64714350E-12-1.53950880E+04 3.66425242E+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
 4
 SC4H8OH 2/12/ 9 THERMC 4H 90 1 0G 300.000 5000.000
 1392.000 41
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1.99145784E-08-3.44416275E-12-3.26698755E+04 2.30901271E+01
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C4H8OOH1-1 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
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1.19327599E-08-1.49401799E-12-5.42740641E+03 2.08094850E+01
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4
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C4H8OOH1-4 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
1400.000 51
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4
C4H8OOH2-1 9/ 1/12 C 4H 90 2 OG 300.000 5000.000
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14 2
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05 3
2.20415677E-08-3.84993017E-12-4.54848974E+03 2.46740872E+01
4

C4H8OOH2-3 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
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4
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4
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4
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1407.000 61
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14 2
-2.87195147E+04-7.96660066E+01 4.97809196E+00 6.30221979E-02-5.08369093E-
05 3
2.14022338E-08-3.61837516E-12-2.33785644E+04 9.92185868E+00
4
C4H8OOH1-3O2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
1403.000 71
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1.94853380E-08-3.10968451E-12-2.32812507E+04 1.19093259E+01
4
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4
C4H8OOH2-1O2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
1407.000 61
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C4H8OOH2-3O2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
1406.000 61

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 1407.000 61
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 NC4KET12 7/19/ 0 THERMC 4H 80 3 OG 300.000 5000.000
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 2.88403536E+04 4
 C2H5COCH2 4/ 3/ 0 THERMC 4H 7O 1 0G 300.000 5000.000
 1383.000 31
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 CH2CH2COCH3 6/21/95 THERC 4H 7O 1 0G 300.000 5000.000 1380.00
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 05 3
 5.07323216E-09-4.99655275E-13-6.15006886E+03 1.93993386E+01
 4
 CH3CHCOCH3 4/ 3/ 0 THERMC 4H 7O 1 0G 300.000 5000.000
 1384.000 31
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 05 3
 8.59326807E-09-1.13188129E-12-1.05247481E+04 2.32952685E+01
 4
 C2H3COCH3 6/19/95 THERMC 4H 6O 1 0G 300.000 5000.000 1386.00
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 05 3
 1.03478392E-08-1.53551381E-12-1.70305379E+04 2.64430799E+01
 4
 CH3CHOOCOCH3 6/27/95 C 4H 7O 3 0G 300.000 5000.000 1393.00
 41
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 14 2
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 05 3
 2.01816805E-08-3.61175600E-12-2.53445178E+04 2.60857480E+01
 4
 CH2CHOHCOCH3 6/27/95 C 4H 7O 3 0G 300.000 5000.000 1394.00
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 14 2
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 05 3

2.16347587E-08-3.75674081E-12-1.89563540E+04 2.71011896E+01
 4
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 14 2
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 05 3
 -1.07815910E-07 4.25781054E-11-2.71198341E+04 4.93592991E+00-
 2.47924787E+04 4
 NC3H7CO 9/27/95 THERMC 4H 70 1 OG 300.000 5000.000 1380.00
 31
 1.30026331E+01 1.63104877E-02-5.57642899E-06 8.65670629E-10-5.02255667E-
 14 2
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 5.48873888E-09-5.35864183E-13-8.58050888E+03 1.64848950E+01
 4
 C3H6CHO-1 9/27/95 THERMC 4H 70 1 OG 300.000 5000.000
 1379.000 31
 1.30322954E+01 1.62418373E-02-5.54388124E-06 8.59723685E-10-4.98459726E-
 14 2
 -6.45915975E+03-3.92399021E+01 2.67672303E+00 3.73064128E-02-2.11281405E-
 05 3
 5.80472681E-09-6.09688236E-13-2.49714183E+03 1.75750933E+01
 4
 C3H6CHO-2 11/15/95 THERMC 4H 70 1 OG 300.000 5000.000
 1682.000 31
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 05 3
 1.67282048E-09 2.62011555E-13-3.79034324E+03 1.74324072E+01
 4
 C3H6CHO-3 11/15/95 THERMC 4H 70 1 OG 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 OG 300.000 5000.000 1400.00
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 14 2
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 1.76564254E-08-3.14365357E-12-1.41717351E+04 2.47118671E+01
 4
 SC3H5CHO 11/15/95 THERC 4H 60 1 OG 300.000 5000.000
 1390.000 21
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 1.33066870E-08-2.17839128E-12-1.60394651E+04 2.37597452E+01
 4

SC3H5CO 11/15/95 THERMC 4H 50 1 0G 300.000 5000.000
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 1.38227925E-08-2.46272017E-12-6.64428100E+02 1.70762023E+01
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 IC4H10 G 8/00C 4 H 10 0 0 G 200.000 6000.00 1000.00
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 1.62354727E+04 4
 IC4H9 T 6/04C 4 H 9 0 0 G 200.000 6000.00 1000.00
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 4.15218608E+03-2.66485099E+01 3.34476784E+00 2.31869650E-02 3.28261040E-
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 8.87422590E+03 4
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 2.11365432E+03 4
 IC4H7 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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 1.65497991E+04 4
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 1380.000 41

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05 3
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4
TC4H8O2H-I 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
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 TC4H9O2H 9/ 1/12 C 4H 100 2 0G 300.000 5000.000
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 1.90926853E+01 2.12697804E-02-7.46252626E-06 1.17841127E-09-6.91795087E-14 2
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 2.22301799E-08-4.00189859E-12-3.12260714E+04 2.37278262E+01
 4
 IC4H7O 4/ 3/ 0 THERMC 4H 70 1 0G 300.000 5000.000
 1386.000 21
 1.33457615E+01 1.61218588E-02-5.44376403E-06 8.38199374E-10-4.83608280E-14 2
 6.11443644E+02-4.36818838E+01 1.74700687E+00 4.07783436E-02-2.44750243E-05 3
 7.06502958E-09-7.51570589E-13 4.86979233E+03 1.94535999E+01
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 IC4H8OH 2/14/95 THERMC 4H 90 1 0G 300.000 5000.000
 1376.000 41
 1.25605997E+01 2.10637488E-02-7.15019648E-06 1.10439262E-09-6.38428695E-14 2
 -1.86203249E+04-3.67889430E+01 3.29612707E+00 3.47649647E-02-1.02505618E-05 3
 -2.04641931E-09 1.18879408E-12-1.45627247E+04 1.58606320E+01
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 IO2C4H8OH 8/23/95 THERMC 4H 90 3 0G 300.000 5000.000
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 1.71759332E-08-2.91842186E-12-3.33881503E+04 1.83381149E+01
 4
 IC3H7CHO 2/22/96 THERMC 4H 80 1 0G 300.000 5000.000
 1391.000 31
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 1.00052945E-08-1.27512074E-12-2.76054737E+04 2.83451139E+01
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 TC3H6CHO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
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 IC3H7CO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
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 14 2
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 8.93548675E-09-1.11327422E-12-9.07755468E+03 2.61991461E+01
 4
 IC4H8OOH-IO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
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 2.24664901E+01 2.09351287E-02-7.44324128E-06 1.18589255E-09-7.00546897E-
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 05 3
 7.79536931E-09-6.21665008E-13-2.22782534E+04 1.52623111E+01
 4
 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
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 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
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 IC4KETII 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
 1387.000 51
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 4
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 1388.000 51
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 1.77145373E-08-2.67265475E-12-4.09366796E+04 2.34844867E+01
 4

IC4H7OH 4/ 8/97 THERMC 4H 80 1 0G 300.000 5000.000
 1384.000 31
 1.35043419E+01 1.78646968E-02-5.99304371E-06 9.18717641E-10-5.28435302E-14 2
 -2.58255688E+04-4.44645715E+01 1.69099899E+00 4.27168891E-02-2.49281695E-05 3
 7.00961522E-09-7.23262828E-13-2.14512334E+04 1.99500833E+01
 4

IC4H6OH 8/19/95 THERMC 4H 70 1 0G 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 7/19/95 THERMC 4H 60 1 0G 300.000 5000.000
 1396.000 21
 1.36203958E+01 1.37917192E-02-4.73370118E-06 7.36655226E-10-4.20097974E-14 2
 -2.00025274E+04-4.73184531E+01 6.27183793E-01 4.66780254E-02-3.74430631E-05 3
 1.58330542E-08-2.73952155E-12-1.57203117E+04 2.16034294E+01
 4

IC3H5CO 4/ 3/ 0 THERMC 4H 50 1 0G 300.000 5000.000
 1397.000 21
 1.30667437E+01 1.16704244E-02-3.99106523E-06 6.19498148E-10-3.59348249E-14 2
 -3.36519344E+03-4.35803090E+01 1.85097069E+00 4.18855846E-02-3.62553731E-05 3
 1.65690659E-08-3.05850846E-12 1.70381441E+02 1.53014433E+01
 4

IC4H7OOH 7/19/95 THERMC 4H 80 2 0G 300.000 5000.000 1392.00
 41
 1.69234564E+01 1.78396769E-02-6.14273279E-06 9.57895028E-10-5.57438304E-14 2
 -2.00040686E+04-5.94746070E+01 2.99117402E+00 5.03349278E-02-3.56280061E-05 3
 1.33952154E-08-2.11053409E-12-1.51095046E+04 1.54537413E+01
 4

IC3H6CO 03/03/95 THERMC 4H 60 1 0G 300.000 5000.000 1397.00
 41
 1.32548232E+01 1.40142787E-02-4.78910215E-06 7.42924342E-10-4.30737566E-14 2
 -2.00529779E+04-4.44810221E+01 2.28039055E+00 4.17016989E-02-3.25089661E-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
 31
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 -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
 IC3H5OH 8/ 1/95 THERMC 3H 60 1 0G 300.000 5000.000 1374.00
 21
 1.07381025E+01 1.31698194E-02-4.41529622E-06 6.77009837E-10-3.89608901E-
 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
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 TC3H6O2HCO 8/ 2/95 THERMC 4H 70 3 0G 300.000 5000.000 1387.00
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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
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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
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 9.13212884E+03-2.25012933E+01 2.88422544E+00 2.42428071E-02-1.14152268E-
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 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
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 14 2

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 1.75737698E-08-2.64896151E-12-6.86582501E+03 3.33781112E+01
 4
 O2C4H8CHO 9/ 7/95 THERMC 5H 90 3 OG 300.000 5000.000 1395.00
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 4
 O2HC4H8CO 9/ 7/95 THERMC 5H 90 3 OG 300.000 5000.000 1394.00
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 -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 OG 300.000 5000.000
 1400.000 71
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 4
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 1394.000 71
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14 2
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4
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14 2
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8.41850668E-09-7.99507437E-13 3.72139256E+03 3.36368332E+01
4
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8.57199815E-09-8.15860099E-13-5.83215050E+03 2.92454905E+01
4
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14 2
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05 3
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 14 2
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 05 3
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 14 2
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 4
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 1396.000 41

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4
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 4
 C5H10OOH2-3 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
 1388.000 61
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 1388.000 61
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 -1.66702092E+04-7.91383677E+01 1.27092209E+00 6.82958985E-02-4.63421243E-
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1.61403755E-08-2.30884220E-12-9.58339948E+03 2.79668173E+01
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C5H100OH2-5 7/19/ 0 THRC 5H 110 2 OG 300.000 5000.000
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4
C5H100OH3-1 7/19/ 0 THRC 5H 110 2 OG 300.000 5000.000
1390.000 61
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05 3
2.26488673E-08-3.77612026E-12-8.22372586E+03 3.02858118E+01
4
C5H100OH3-2 7/19/ 0 THRC 5H 110 2 OG 300.000 5000.000
1388.000 61
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-1.66702092E+04-7.91383677E+01 1.27092209E+00 6.82958985E-02-4.63421243E-
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1.17684771E-08-1.26029870E-12-2.80943137E+04 4.58617150E+01
4
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4

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 1.76515898E-08-2.56653255E-12-2.03198734E+04 4.22612571E+01
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 4
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 1387.000 71
 2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-
 14 2
 -3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-
 05 3
 2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
 4
 C5H10OOH1-4O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
 1387.000 71
 2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-
 14 2
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 05 3
 2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
 4
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 1385.000 71
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 2.23236523E-08-3.71501383E-12-2.43447483E+04 2.35135259E+01
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 1387.000 71
 2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-
 14 2
 -3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-
 05 3
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 4
 C5H10OOH2-3O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
 1389.000 71

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 3.07497216E-08-5.51132533E-12-2.90970365E+04 2.50297599E+01
 4
 C5H10OOH2-4O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
 1389.000 71
 2.62850175E+01 2.43678422E-02-8.50101950E-06 1.33736519E-09-7.83075048E-
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 05 3
 2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
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 C5H10OOH3-1O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
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 2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-
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 2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
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 C5H10OOH3-2O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
 1389.000 71
 2.62850175E+01 2.43678422E-02-8.50101950E-06 1.33736519E-09-7.83075048E-
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 05 3
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 4
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 05 3
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 NC5KET13 7/19/ 0 THERMC 5H 100 3 OG 300.000 5000.000
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 14 2
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 2.12906293E-08-3.56676536E-12-4.29988725E+04 2.14543054E+01
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 14 2
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 1.29220662E-08-1.89791227E-12-4.47703435E+04 1.29580830E+01
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 2.36744270E-08-3.89094338E-12-4.57495597E+04 3.32799795E+01
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 2.00741570E-08-3.28568948E-12-4.66368524E+04 2.29520202E+01
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 1.58213340E-08-2.38800145E-12-4.43093682E+04 2.11180678E+01
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 NC5KET31 7/19/ 0 THERMC 5H 100 3 OG 300.000 5000.000
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 14 2
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 1.85573234E-08-3.11995924E-12-4.46228757E+04 1.89760116E+01
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 NC5KET32 7/19/ 0 THERMC 5H 100 3 OG 300.000 5000.000
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 4
 C5H10OH-1 1/14/99 THERMC 5H 110 1 0G 300.000 5000.000
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 5.54684921E-09 1.10578801E-14-1.48168651E+04 2.93877119E+01
 4
 C5H10OH-2 1/14/99 THERMC 5H 110 1 0G 300.000 5000.000
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 14 2
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 1.16488887E-08-1.41506375E-12-1.70158316E+04 3.00652481E+01
 4
 O2C5H10OH-1 1/14/99 THRMC 5H 110 3 0G 300.000 5000.000
 1395.000 61
 2.06059936E+01 2.61750874E-02-8.92270421E-06 1.38184638E-09-8.00235870E-
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 1.81238720E-08-2.90871344E-12-3.44822614E+04 2.22673007E+01
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 1398.000 61
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 2.24979959E-08-3.79045894E-12-3.66230283E+04 2.45460172E+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-T 12/ 5/12 THERMC 6H 9 0 0G 300.000 5000.000
 1399.000 21
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 14 2
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 1.77756829E-08-2.95693412E-12 3.62924888E+04 3.28081912E+01
 4
 C6H9-S 12/ 5/12 THERMC 6H 9 0 0G 300.000 5000.000
 1396.000 31
 1.62958005E+01 2.11783659E-02-7.25674435E-06 1.12780699E-09-6.54746480E-
 14 2
 3.20417675E+04-5.73406449E+01-6.12878674E-01 6.32013662E-02-4.85579869E-
 05 3
 2.01072289E-08-3.46242218E-12 3.77343371E+04 3.26952798E+01
 4

C6H9O-2 12/ 5/12 THERMC 6H 90 1 0G 300.000 5000.000
1381.000 41
1.99353187E+01 2.10902650E-02-7.42714919E-06 1.17580440E-09-6.91504434E-
14 2
7.67409302E+03-7.62069031E+01-7.85602487E-02 6.81070170E-02-5.11911414E-
05 3
2.04828658E-08-3.45141659E-12 1.47423639E+04 3.14323712E+01
4
C6H6 G 6/01C 6H 6 0 0G 200.000 6000.000
1000.000 1
1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-
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
C6H5CH3 L 6/87C 7H 8 0 0G 200.000 6000.000 1000.
1
0.12940034E+02 0.26691287E-01-0.96838505E-05 0.15738629E-08-0.94663601E-
13 2
-0.69764908E+03-0.46728785E+02 0.16152663E+01 0.21099438E-01 0.85366018E-
04 3
-0.13261066E-06 0.55956604E-10 0.40756300E+04 0.20282210E+02
0.60135835E+04 4
C6H5CH2 IU3/03C 7.H 7. 0. 0.G 250.000 6000.000 1000.
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0.14723052E+02 0.23034244E-01-0.84847359E-05 0.13916962E-08-0.84247967E-
13 2
0.17990189E+05-0.55950989E+02-0.12303836E+01 0.48986376E-01 0.13815518E-
04 3
-0.62587233E-07 0.31595731E-10 0.23192877E+05 0.30555495E+02
0.25016622E+05 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
4
CC3H4 T12/81C 3H 4 0 0G 300.000 5000.00 1000.00
1
0.66999931E+01 0.10357372E-01-0.34551167E-05 0.50652949E-09-0.26682276E-
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
C4H4 H6W/94C 4H 4 0 0G 300.000 3000.00 1000.00
1
0.66507092E+01 0.16129434E-01-0.71938875E-05 0.14981787E-08-0.11864110E-
12 2
0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-
04 3
0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02
4
C4H3-I AB1/93C 4H 3 0 0G 300.000 3000.00 1000.00
1

0.90978165E+01 0.92207119E-02-0.33878441E-05 0.49160498E-09-0.14529780E-
 13 2
 0.56600574E+05-0.19802597E+02 0.20830412E+01 0.40834274E-01-0.62159685E-
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 0.51679358E-07-0.17029184E-10 0.58005129E+05 0.13617462E+02
 4
 C4H612 A 8/83C 4H 6 0 0G 300. 3000. 1000.0
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 0.1781557E 02 -0.4257502E-02 0.1051185E-04 -0.4473844E-08 0.5848138E-
 12 2
 0.1267342E 05 -0.6982662E 02 0.1023467E 01 0.3495919E-01 -0.2200905E-
 04 3
 0.6942272E-08 -0.7879187E-12 0.1811799E 05 0.1975066E 02
 0.1950807E+05 4
 C6H5 T04/02C 6H 5 0 0G 200.000 6000.000 1000.
 1
 1.08444762E+01 1.73212473E-02-6.29233249E-06 1.02369961E-09-6.16216828E-
 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
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 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-
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 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
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 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
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 12 2
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 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

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05 3
1.45472667E-08-2.65454288E-12 1.47887943E+03 1.67433588E+01
4
CH2CHCHCHO T03/97C 4H 50 1 0G 200.000 6000.000 1000.0
1
8.90967920E+00 1.34364140E-02-7.62977390E-07-1.69114810E-09 2.95540440E-
13 2
1.48898740E+03-1.79662460E+01-1.08199860E+00 3.64929760E-02-1.52255950E-
05 3
-5.62607170E-18 2.16113750E-21 3.56713230E+03 3.27142550E+01
4.73074990E+03 4
C4H6O25 T 3/97C 4H 60 1 0G 200.000 5000.000 1000.0
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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 A 8/83C 4H 60 1 0G 300. 3000. 1000.0
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12 2
1.75352252E+03 5.17190420E+01 7.97985440E-01 3.44034320E-02-1.24598510E-
05 3
-5.18062790E-18 1.99359540E-21-6.48927540E+02 2.18896980E+01
1.00654250E+03 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-
06 3
-1.01525890E-08 3.05010094E-12 1.59213397E+04 1.39603990E+01
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-
05 3
-1.26219194E-07 5.23991321E-11-1.02787872E+04 1.45722395E+01-
1.30831522E+04 4
CH3CHCHCHO T 5/92C 4H 60 1 0G 298.150 3000.0 1000.0
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1.98794540E+01-2.09130550E-02 4.45360508E-05-2.60374870E-08 4.86836120E-
12 2
-1.95278768E+04-6.87200320E+01-1.55577660E+00 4.09640630E-02-1.69868810E-
05 3

-6.00928140E-18 2.31368530E-21-1.41394920E+04 3.74707580E+01-
1.29340710E+04 4
C4H4O T03/97C 4H 4O 1 0G 200.000 6000.0 1000.0
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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 4O 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 C 5 H 5 G250.000 5000.000 995.00
1
! 9.56337366E+00 1.74277088E-02-6.86085196E-06 1.23916759E-09-
8.41087417E-14 2
! 2.81845298E+04-2.81373712E+01 5.16970848E-01 2.76670206E-02
2.33775674E-05 3
!-5.70072196E-08 2.66905847E-11 3.12367412E+04 2.17162771E+01
3.27225830E+04 4
!C5H6 C 5 H 6 G250.000 5000.000 995.00
1
! 8.54224876E+00 2.14442757E-02-8.49864028E-06 1.54187677E-09-
1.04980310E-13 2
! 1.27177699E+04-2.43630856E+01 2.02640754E-01 2.16857125E-02
4.89543516E-05 3
!-8.47163463E-08 3.67450866E-11 1.59781268E+04 2.38173249E+01
1.72796300E+04 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
 HOC6H4OH 4/ 9/ 9 THERMC 6H 60 2 0G 300.000 5000.000
 1405.000 21
 2.31394847E+01 1.31873680E-02-4.49072464E-06 6.95268891E-10-4.02643108E-
 14 2

-4.25885990E+04-1.02692352E+02-8.68529064E+00 1.17282933E-01-1.33754802E-
 04 3
 7.16697462E-08-1.44385730E-11-3.44903827E+04 5.77087257E+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
 2.80683553E-08-4.92279426E-12 6.73402222E+03 4.09349895E+01
 4
 O-OC6H5OJ WKM C 60 2H 5 0G 300.000 5000.000
 1400.000 01
 1.84625733E+01 1.57607263E-02-5.44671499E-06 8.51765760E-10-4.96759541E-
 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-
 14 2
 7.60582726E+03-5.43599625E+01-2.18492198E-01 5.92100223E-02-5.89241174E-
 05 3

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
 1402.000 11
 1.07482537E+01 6.19822688E-03-2.06130981E-06 3.14418872E-10-1.80309517E-
 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 0G 300.000 3500.000 1500.00
 1
 1.19961781E+01 1.34287065E-02-5.90045309E-06 1.22553862E-09-9.86114716E-
 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
 OC5H70 1/22/ 9 WKM C 5H 70 2 0G 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 0G 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*CC 3/1/95 Z&B C 5H 8 0 0G 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 0G 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 OG 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 OG 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 OG 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 OG 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 OG 300.00 5000.00 1000.00
 1
 6.81339897E+00 8.05827723E-03-3.11728612E-06 5.54590896E-10-3.71804255E-14 2
 1.31583034E+04-1.09863525E+01 5.62397968E-01 2.64598620E-02-2.28453705E-05 3
 9.14478695E-09-1.06711936E-12 1.48374643E+04 2.10439544E+01
 4

O2CCHOOJ Z&B C 2H 10 4 OG 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 OG 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 OG 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
 CH3CHCHO 12/ 1/99 THERMC 3H 50 1 0G 300.000 5000.000
 1385.000 21
 1.02647528E+01 1.17295061E-02-4.06267561E-06 6.36086751E-10-3.71220190E-
 14 2
 -7.25910488E+03-2.91646638E+01 1.54196914E+00 3.03297391E-02-1.88922690E-
 05 3
 5.92263358E-09-7.53762316E-13-4.01761098E+03 1.83707011E+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
 SC3H4OH-1 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1410.000 21
 1.25628085E+01 8.58651176E-03-2.72582845E-06 4.01908549E-10-2.24787697E-
 14 2
 3.96526183E+03-4.16107625E+01 2.55744565E-01 4.74882684E-02-4.94984843E-
 05 3
 2.53799319E-08-4.97487174E-12 7.19097870E+03 2.08288803E+01
 4
 IC3H5O 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1397.000 21
 1.23529178E+01 9.83087082E-03-3.37836468E-06 5.26074995E-10-3.05827836E-
 14 2

1.05079663E+03-4.24057711E+01 6.71872962E-01 4.46259031E-02-4.42421428E-
 05 3
 2.23584078E-08-4.41548328E-12 4.43070338E+03 1.77897863E+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
 C6H11 C 6 H 11 G100.000 5000.000 1258.20
 1
 1.13629241E+01 3.32027833E-02-1.26820422E-05 2.25518835E-09-1.52582242E-
 13 2
 1.21188102E+04-2.80854603E+01 2.64055302E+00 4.43747867E-02-6.26124800E-
 06 3
 -1.16062670E-08 4.67988886E-12 1.56242965E+04 2.12065144E+01
 4
 H2COCOCH3 7/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1412.000 21
 3.79062737E+01 5.42971051E-03-3.33938604E-06 8.33177683E-10-7.95831961E-
 14 2
 -2.09703405E+04-1.40902518E+02 4.11384586E+01-7.62663758E-05-3.51139955E-
 08 3
 -1.14125528E-12-3.30331004E-15-2.24026434E+04-1.59157172E+02
 4
 CCYCOO 7/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1398.000 21
 1.52842170E+01 9.91133864E-03-3.41434716E-06 5.32813858E-10-3.10289585E-
 14 2
 1.41164858E+03-5.24636435E+01 2.55262174E+00 4.36110094E-02-3.81896570E-
 05 3
 1.69947150E-08-3.01394020E-12 5.41657441E+03 1.44748296E+01
 4
 TC3H5OO 6/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1398.000 21
 1.44892862E+01 1.06189587E-02-3.66414488E-06 5.72282956E-10-3.33427783E-
 14 2
 -2.14964368E+03-4.82072152E+01 2.32747386E+00 4.28458215E-02-3.71917675E-
 05 3
 1.66530071E-08-2.99207781E-12 1.69979772E+03 1.57682500E+01
 4
 cy(CJCCCC) C 5 H 9 G 3E+02 1E+03 6E+02
 1
 -1.22792398E+00 3.58055323E-02 3.35582231E-05-7.13287163E-08 3.18281993E-
 11 2
 1.15391896E+04 3.14847993E+01-1.22792398E+00 3.58055323E-02 3.35582231E-
 05 3
 -7.13287163E-08 3.18281993E-11 1.15391896E+04 3.14847993E+01
 4
 C*CCCC*O C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 5.73084267E+00 1.99430238E-02 3.77135520E-05-5.82387829E-08 2.31845126E-
 11 2
 -1.50460165E+04 5.46952522E+00 5.73084267E+00 1.99430238E-02 3.77135520E-
 05 3

-5.82387829E-08 2.31845126E-11-1.50460165E+04 5.46952522E+00
4
C6H9O4r_Olef_13 C 6 O 4 H 9 G 3E+02 1E+03 6E+02
1
-3.36596053E+00 1.37074756E-01-2.02289794E-04 1.64104739E-07-5.44542443E-
11 2
1.43592115E+03 4.48463958E+01-3.36596053E+00 1.37074756E-01-2.02289794E-
04 3
1.64104739E-07-5.44542443E-11 1.43592115E+03 4.48463958E+01
4
C4H8O_Olef_1 C 4 O 1 H 8 G 3E+02 1E+03 6E+02
1
7.58655279E-01 5.60555489E-02-5.15820383E-05 2.61810966E-08-5.27185175E-
12 2
-2.25280895E+04 2.21099822E+01 7.58655279E-01 5.60555489E-02-5.15820383E-
05 3
2.61810966E-08-5.27185175E-12-2.25280895E+04 2.21099822E+01
4
C6H10_Olef_6 C 6 H 10 G 3E+02 1E+03 6E+02
1
2.73653094E+00 3.46681417E-02 3.81285890E-05-7.58567975E-08 3.30951942E-
11 2
3.36056675E+03 1.48044786E+01 2.73653094E+00 3.46681417E-02 3.81285890E-
05 3
-7.58567975E-08 3.30951942E-11 3.36056675E+03 1.48044786E+01
4
C5H6O_Olef_1 C 5 O 1 H 6 G 3E+02 1E+03 6E+02
1
-5.60395793E+00 9.66315214E-02-1.31318303E-04 9.62748696E-08-2.87375144E-
11 2
-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
C6H10_Olef_3 C 6 H 10 G 3E+02 1E+03 6E+02
1
5.58428633E+00 2.41515267E-02 4.24982128E-05-6.75738305E-08 2.73631976E-
11 2
6.19830319E+03 4.44605027E+00 5.58428633E+00 2.41515267E-02 4.24982128E-
05 3
-6.75738305E-08 2.73631976E-11 6.19830319E+03 4.44605027E+00
4
C6H11r_Olef_7 C 6 H 11 G 3E+02 1E+03 6E+02
1
4.91319024E+00 3.21131405E-02 2.96633475E-05-5.66811380E-08 2.37985959E-
11 2
1.60010795E+04 6.48426297E+00 4.91319024E+00 3.21131405E-02 2.96633475E-
05 3
-5.66811380E-08 2.37985959E-11 1.60010795E+04 6.48426297E+00
4
C4H8O_Olef_2 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

C6H9O2r_Olef_6 C 6 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 1.59238455E+00 8.20483692E-02-9.84081726E-05 7.38278027E-08-2.40039796E-
 11 2
 1.34795747E+04 2.02952685E+01 1.59238455E+00 8.20483692E-02-9.84081726E-
 05 3
 7.38278027E-08-2.40039796E-11 1.34795747E+04 2.02952685E+01
 4
 Ccy(CCCJCC) C 6 H 11 G 3E+02 1E+03 6E+02
 1
 -2.22787683E+00 5.78990732E-02-3.87248974E-06-3.52629373E-08 1.82890749E-
 11 2
 7.49823810E+03 3.56420040E+01-2.22787683E+00 5.78990732E-02-3.87248974E-
 06 3
 -3.52629373E-08 1.82890749E-11 7.49823810E+03 3.56420040E+01
 4
 CJcy(CCC*CC) C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -2.31922889E+00 5.78306944E-02-2.86582652E-05 2.09899409E-09 1.67642185E-
 12 2
 2.51453217E+04 3.72159447E+01-2.31922889E+00 5.78306944E-02-2.86582652E-
 05 3
 2.09899409E-09 1.67642185E-12 2.51453217E+04 3.72159447E+01
 4
 Ccy(CCJC*CC) C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -3.04279127E+00 5.78353198E-02-2.42108815E-05-3.49441632E-09 3.78795404E-
 12 2
 1.62023610E+04 3.80639706E+01-3.04279127E+00 5.78353198E-02-2.42108815E-
 05 3
 -3.49441632E-09 3.78795404E-12 1.62023610E+04 3.80639706E+01
 4
 C6H10O_Olef_1 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
 1
 4.57438068E+00 3.65908994E-02 2.11709609E-05-4.91819629E-08 2.11832236E-
 11 2
 -2.24140577E+04 1.10694676E+01 4.57438068E+00 3.65908994E-02 2.11709609E-
 05 3
 -4.91819629E-08 2.11832236E-11-2.24140577E+04 1.10694676E+01
 4
 C*CCJCCC C 6 H 11 G 3E+02 1E+03 6E+02
 1
 -1.10439009E-02 6.24600000E-02-3.67600000E-05 8.79399999E-09-1.69199999E-
 13 2
 8.94800000E+03 2.90700000E+01-1.10439009E-02 6.24600000E-02-3.67600000E-
 05 3
 8.79399999E-09-1.69199999E-13 8.94800000E+03 2.90700000E+01
 4
 C6H11Or_Olef_48 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 5.64372553E+00 4.09515397E-02 9.61332366E-06-3.70492310E-08 1.68632335E-
 11 2
 -3.89992551E+03 7.06581167E+00 5.64372553E+00 4.09515397E-02 9.61332366E-
 06 3
 -3.70492310E-08 1.68632335E-11-3.89992551E+03 7.06581167E+00
 4
 Ccy(CC*CC*C) C 6 H 8 G 3E+02 1E+03 6E+02
 1

-3.80606110E+00 6.19045057E-02-2.56010408E-05-1.61860299E-08 1.28769566E-11 2
 1.22752214E+04 4.17807157E+01-3.80606110E+00 6.19045057E-02-2.56010408E-05 3
 -1.61860299E-08 1.28769566E-11 1.22752214E+04 4.17807157E+01 4
 C6H11Or_Olef_35 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 5.51700664E+00 3.83413374E-02 1.83776953E-05-4.68572798E-08 2.05427945E-11 2
 -4.47833111E+03 8.81979897E+00 5.51700664E+00 3.83413374E-02 1.83776953E-05 3
 -4.68572798E-08 2.05427945E-11-4.47833111E+03 8.81979897E+00 4
 C6H9Or_Olef C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -4.13421360E+00 9.24569586E-02-9.13689000E-05 4.44248819E-08-7.61018131E-12 2
 8.95363789E+02 4.75267157E+01-4.13421360E+00 9.24569586E-02-9.13689000E-05 3
 4.44248819E-08-7.61018131E-12 8.95363789E+02 4.75267157E+01 4
 C*CC*CC*C C 6 H 8 G 3E+02 1E+03 6E+02
 1
 -2.04253243E+00 5.57575035E-02 2.72924219E-06-5.61491470E-08 2.99604618E-11 2
 1.88694134E+04 3.48687906E+01-2.04253243E+00 5.57575035E-02 2.72924219E-06 3
 -5.61491470E-08 2.99604618E-11 1.88694134E+04 3.48687906E+01 4
 C6H11Or_Olef_4 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 5.48305313E+00 3.88252391E-02 2.02826767E-05-5.05660696E-08 2.21673283E-11 2
 -7.26156105E+03 8.05018893E+00 5.48305313E+00 3.88252391E-02 2.02826767E-05 3
 -5.05660696E-08 2.21673283E-11-7.26156105E+03 8.05018893E+00 4
 C6H11r_Olef 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
 C*CC(*O)CC*C C 6 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 -1.63529790E+00 9.00550908E-02-1.20540171E-04 9.53129857E-08-3.10170751E-11 2
 -7.53473206E+03 3.51341790E+01-1.63529790E+00 9.00550908E-02-1.20540171E-04 3
 9.53129857E-08-3.10170751E-11-7.53473206E+03 3.51341790E+01 4
 C6H11r_Olef_2 C 6 H 11 G 3E+02 1E+03 6E+02
 1
 5.97921142E+00 1.99257385E-02 5.83270434E-05-8.34607225E-08 3.28025556E-11 2

1.45047511E+04 3.50364675E+00 5.97921142E+00 1.99257385E-02 5.83270434E-
05 3
-8.34607225E-08 3.28025556E-11 1.45047511E+04 3.50364675E+00
4
C*CCCy(COC) C 6 O 1 H 10 G 3E+02 1E+03 6E+02
1
1.16275494E+01-1.09821617E-02 1.38333935E-04-1.67265595E-07 6.34445206E-
11 2
-6.67133561E+03-2.17737614E+01 1.16275494E+01-1.09821617E-02 1.38333935E-
04 3
-1.67265595E-07 6.34445206E-11-6.67133561E+03-2.17737614E+01
4
Ccy(C*CC*CC) C 6 H 8 G 3E+02 1E+03 6E+02
1
-2.22888333E+00 5.02723009E-02-4.95614944E-06-3.01409958E-08 1.59405864E-
11 2
1.07062578E+04 3.63680140E+01-2.22888333E+00 5.02723009E-02-4.95614944E-
06 3
-3.01409958E-08 1.59405864E-11 1.07062578E+04 3.63680140E+01
4
C6H9r_R5_9 C 6 H 9 G 3E+02 1E+03 6E+02
1
-1.10877088E+00 4.99289259E-02-1.37269628E-05-9.02483884E-09 4.65887014E-
12 2
1.52455893E+04 3.07005281E+01-1.10877088E+00 4.99289259E-02-1.37269628E-
05 3
-9.02483884E-09 4.65887014E-12 1.52455893E+04 3.07005281E+01
4
C6H11Or_Olef_42 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
5.97185474E+00 4.00818232E-02 1.27463533E-05-4.12617060E-08 1.86442755E-
11 2
-3.38869012E+03 5.89633118E+00 5.97185474E+00 4.00818232E-02 1.27463533E-
05 3
-4.12617060E-08 1.86442755E-11-3.38869012E+03 5.89633118E+00
4
C6H11Or_Olef_23 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
-1.06629276E+00 8.20468024E-02-6.69552937E-05 2.49039930E-08-1.93837830E-
12 2
-1.29368072E+04 3.16778455E+01-1.06629276E+00 8.20468024E-02-6.69552937E-
05 3
2.49039930E-08-1.93837830E-12-1.29368072E+04 3.16778455E+01
4
C6H11Or_Olef_32 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
6.09825627E+00 3.62617691E-02 2.51649644E-05-5.44962545E-08 2.34521848E-
11 2
-1.22431048E+04 4.60544458E+00 6.09825627E+00 3.62617691E-02 2.51649644E-
05 3
-5.44962545E-08 2.34521848E-11-1.22431048E+04 4.60544458E+00
4
C6H9r_R5_10 C 6 H 9 G 3E+02 1E+03 6E+02
1
-1.10877088E+00 4.99289259E-02-1.37269628E-05-9.02483884E-09 4.65887014E-
12 2
1.52455893E+04 2.89087686E+01-1.10877088E+00 4.99289259E-02-1.37269628E-
05 3

-9.02483884E-09 4.65887014E-12 1.52455893E+04 2.89087686E+01
 4
 C6H11Or_Olef_49 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 9.33560154E-01 7.31458066E-02-5.89812961E-05 2.54760165E-08-4.16061532E-
 12 2
 -5.61234329E+03 2.58326720E+01 9.33560154E-01 7.31458066E-02-5.89812961E-
 05 3
 2.54760165E-08-4.16061532E-12-5.61234329E+03 2.58326720E+01
 4
 cy(C*CCC*CC) C 6 H 8 G 3E+02 1E+03 6E+02
 1
 1.90182000E+00 1.48193940E-02 9.13121941E-05-1.34589490E-07 5.59079720E-
 11 2
 1.13167500E+04 1.74071510E+01 1.90182000E+00 1.48193940E-02 9.13121941E-
 05 3
 -1.34589490E-07 5.59079720E-11 1.13167500E+04 1.74071510E+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
 C6H8O_Olef_14 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 -4.50220986E+00 1.22762588E-01-2.07723564E-04 1.89125654E-07-6.64313620E-
 11 2
 -1.11667516E+04 4.42908842E+01-4.50220986E+00 1.22762588E-01-2.07723564E-
 04 3
 1.89125654E-07-6.64313620E-11-1.11667516E+04 4.42908842E+01
 4
 C6H9Or_Olef_18 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 8.09207395E+00 2.46495439E-02 2.52111501E-05-4.02875655E-08 1.50628228E-
 11 2
 1.46673378E+04-3.94832544E+00 8.09207395E+00 2.46495439E-02 2.52111501E-
 05 3
 -4.02875655E-08 1.50628228E-11 1.46673378E+04-3.94832544E+00
 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
 C4H4O_Olef C 4 O 1 H 4 G 3E+02 1E+03 6E+02
 1
 8.42832571E-01 3.79161482E-02-2.84694471E-05 9.01868685E-09-2.00243511E-
 13 2
 1.49815379E+03 2.13452370E+01 8.42832571E-01 3.79161482E-02-2.84694471E-
 05 3
 9.01868685E-09-2.00243511E-13 1.49815379E+03 2.13452370E+01
 4

C6H11Or_Olef_27 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 1.33534277E+00 6.56460918E-02-2.46719373E-05-1.98299614E-08 1.46160500E-
 11 2
 -5.93996456E+03 2.41644967E+01 1.33534277E+00 6.56460918E-02-2.46719373E-
 05 3
 -1.98299614E-08 1.46160500E-11-5.93996456E+03 2.41644967E+01
 4
 C*CCJCC C 5 H 9 G 3E+02 1E+03 6E+02
 1
 -2.78104001E-01 5.27800000E-02-3.34800000E-05 1.00400000E-08-9.55400002E-
 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
 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
 C5H7r_Olef C 5 H 7 G 3E+02 1E+03 6E+02
 1
 8.99434536E-01 3.99911400E-02-1.29802043E-06-3.13903171E-08 1.68389571E-
 11 2
 3.77859573E+04 2.10962672E+01 8.99434536E-01 3.99911400E-02-1.29802043E-
 06 3
 -3.13903171E-08 1.68389571E-11 3.77859573E+04 2.10962672E+01
 4
 C6H11r_Olef_1 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-
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 4
 C5H9O2r_Olef C 5 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 1.85183265E+00 7.30670827E-02-7.92060455E-05 5.45288730E-08-1.71765380E-
 11 2
 7.09055570E+03 2.22191254E+01 1.85183265E+00 7.30670827E-02-7.92060455E-
 05 3
 5.45288730E-08-1.71765380E-11 7.09055570E+03 2.22191254E+01
 4
 C5H8O_Olef_7 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
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 05 3
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-6.18432096E+00 1.67968658E-01-3.14505460E-04 2.98076140E-07-1.07020334E-10 2
-2.04278235E+04 5.29775801E+01-6.18432096E+00 1.67968658E-01-3.14505460E-04 3
2.98076140E-07-1.07020334E-10-2.04278235E+04 5.29775801E+01
4
C6H11Or_Olef_18 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
2.57757998E+00 6.76299447E-02-4.40472281E-05 7.20800905E-09 3.45535701E-12 2
-4.83083317E+03 1.53372547E+01 2.57757998E+00 6.76299447E-02-4.40472281E-05 3
7.20800905E-09 3.45535701E-12-4.83083317E+03 1.53372547E+01
4
C6H11Or_Olef_13 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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4.53008332E+00 4.72339989E-02 2.82958399E-06-3.69463133E-08 1.85557776E-11 2
-4.46774887E+03 9.39386291E+00 4.53008332E+00 4.72339989E-02 2.82958399E-06 3
-3.69463133E-08 1.85557776E-11-4.46774887E+03 9.39386291E+00
4
C4H7Or_Olef_7 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
1
1.09956584E+00 5.03615921E-02-4.43624168E-05 2.11935557E-08-3.88399422E-12 2
-3.44651804E+03 2.07681165E+01 1.09956584E+00 5.03615921E-02-4.43624168E-05 3
2.11935557E-08-3.88399422E-12-3.44651804E+03 2.07681165E+01
4
C6H11Or_Olef_34 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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-1.22431048E+04 3.50683229E+00 6.09825627E+00 3.62617691E-02 2.51649644E-05 3
-5.44962545E-08 2.34521848E-11-1.22431048E+04 3.50683229E+00
4
C6H11Or_Olef_7 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
1
5.57614916E+00 3.65191061E-02 2.45774136E-05-5.35721526E-08 2.29100771E-11 2
-8.47011648E+03 6.38061722E+00 5.57614916E+00 3.65191061E-02 2.45774136E-05 3
-5.35721526E-08 2.29100771E-11-8.47011648E+03 6.38061722E+00
4
C6H8O_Olef_7 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
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6.24473200E+03-2.09272662E-01 5.61337557E+00 2.50558710E-02 6.52184817E-05 3
-1.09978385E-07 4.70297696E-11 6.24473200E+03-2.09272662E-01
4
C6H9O4r_Olef_1 C 6 O 4 H 9 G 3E+02 1E+03 6E+02
1
-4.64105519E+00 1.56541139E-01-2.58960638E-04 2.24826567E-07-7.68241870E-11 2

2.75433280E+03 4.74609444E+01-4.64105519E+00 1.56541139E-01-2.58960638E-
 04 3
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 CJcy(CC*CC*C) C 6 H 7 G 3E+02 1E+03 6E+02
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 12 2
 3.75520270E+04 4.55505671E+01-4.27005533E+00 6.71079263E-02-4.88024296E-
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 C*CCCC*O C 6 O 1 H 10 G 3E+02 1E+03 6E+02
 1
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 11 2
 1.44426408E+04 3.37711038E+01-9.58819714E-01 9.68440651E-02-1.27181886E-
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 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
 C6H10O2_Olef_2 C 6 O 2 H 10 G 3E+02 1E+03 6E+02
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 11 2
 -6.62326083E+03 3.99270685E+01-3.04216718E+00 1.06322745E-01-1.16564287E-
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 6.96355249E-08-1.78113930E-11-6.62326083E+03 3.99270685E+01
 4
 C*cy(CCJCC*C) C 6 H 7 G 3E+02 1E+03 6E+02
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 12 2
 2.84697094E+04 4.35630166E+01-4.22275006E+00 6.64245043E-02-4.23658937E-
 05 3
 1.01738404E-09 6.92627527E-12 2.84697094E+04 4.35630166E+01
 4
 C6H9r_Olef C 6 H 9 G 3E+02 1E+03 6E+02
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 12 2
 3.05600000E+04 3.92300000E+01-2.24554000E+00 7.08000000E-02-5.60900000E-
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2.17600000E-08-3.11900000E-12 3.05600000E+04 3.92300000E+01
 4
 C6H11Or_Olef_40 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 12 2
 -5.89566532E+03 1.82220309E+01 2.92403283E+00 5.82679542E-02-2.21007901E-
 05 3
 -1.25354937E-08 9.79892263E-12-5.89566532E+03 1.82220309E+01
 4
 C6H11Or_Olef_26 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 2.34268021E+00 5.66965575E-02-7.57927548E-06-3.30785994E-08 1.83774100E-
 11 2
 -7.46065879E+03 2.07123675E+01 2.34268021E+00 5.66965575E-02-7.57927548E-
 06 3
 -3.30785994E-08 1.83774100E-11-7.46065879E+03 2.07123675E+01
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 C*cy(CC*CCC) C 6 H 8 G 3E+02 1E+03 6E+02
 1
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 11 2
 1.30996093E+04 4.38718440E+01-4.05726286E+00 6.59702270E-02-5.79702878E-
 05 3
 3.55970710E-08-1.11111402E-11 1.30996093E+04 4.38718440E+01
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 C6H11Or_Olef_55 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 11 2
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 05 3
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 C6H9O4r_Olef_7 C 6 O 4 H 9 G 3E+02 1E+03 6E+02
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 04 3
 1.82778288E-07-6.45929517E-11 4.21850282E+03 3.00805766E+01
 4
 C6H9O2r_Olef_4 C 6 O 2 H 9 G 3E+02 1E+03 6E+02
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 11 2
 1.16820861E+04 3.99043315E+01-3.07799982E+00 1.04925804E-01-1.27304624E-
 04 3
 8.61463129E-08-2.46502739E-11 1.16820861E+04 3.99043315E+01
 4
 C6H10O_Olef_9 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
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 3.64236006E+00 4.19323830E-02 1.01782518E-05-3.89963808E-08 1.76963539E-
 11 2
 -1.83486062E+04 1.60976022E+01 3.64236006E+00 4.19323830E-02 1.01782518E-
 05 3
 -3.89963808E-08 1.76963539E-11-1.83486062E+04 1.60976022E+01
 4

C2H3Or_Olef C 2 O 1 H 3 G 3E+02 1E+03 6E+02
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 12 2
 1.27428672E+04 2.16576043E+01 4.22756795E-01 3.31561170E-02-4.30026060E-
 05 3
 2.95165767E-08-8.05890719E-12 1.27428672E+04 2.16576043E+01
 4
 C6H11Or_Olef_14 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -1.92096692E+04 1.09738696E+01 3.97039191E+00 4.42810316E-02 1.94200875E-
 05 3
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 13 2
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 C2H4O3 C 2 O 3 H 4 G 3E+02 1E+03 6E+02
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 12 2
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 4
 C4H7Or_Olef_2 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 2.15203271E+00 4.55440861E-02-3.23987651E-05 8.98688465E-09 4.45243489E-
 13 2
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 05 3
 8.98688465E-09 4.45243489E-13-9.49214941E+03 1.66613820E+01
 4
 C5H9r_Olef_2 C 5 H 9 G 3E+02 1E+03 6E+02
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 3.48893924E+00 3.31654413E-02 6.89246523E-06-2.90277034E-08 1.33172425E-
 11 2
 2.51901465E+04 1.16493696E+01 3.48893924E+00 3.31654413E-02 6.89246523E-
 06 3
 -2.90277034E-08 1.33172425E-11 2.51901465E+04 1.16493696E+01
 4
 C6H11Or_Olef_16 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 1.10541423E+00 7.64463328E-02-6.20953837E-05 2.27035103E-08-1.38068807E-
 12 2
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 05 3
 2.27035103E-08-1.38068807E-12-4.14749202E+03 2.15114539E+01
 4
 C6H10O2_Olef_15 C 6 O 2 H 10 G 3E+02 1E+03 6E+02
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 4
 C5H8O_Olef_5 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -1.54565135E+04 3.48111405E+01-2.04134233E+00 6.44004351E-02-2.78742137E-
 05 3
 -2.14930623E-08 1.67992691E-11-1.54565135E+04 3.48111405E+01
 4
 C6H11O2r_1 C 6 O 2 H 11 G 3E+02 1E+03 6E+02
 1
 2.81761065E+00 7.39225819E-02-5.98276911E-05 2.93641419E-08-7.32878259E-
 12 2
 6.20501828E+03 1.98353016E+01 2.81761065E+00 7.39225819E-02-5.98276911E-
 05 3
 2.93641419E-08-7.32878259E-12 6.20501828E+03 1.98353016E+01
 4
 C6H8O_Olef_9 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -8.56431436E+03 4.16902777E+01-3.87501633E+00 9.63612650E-02-1.13661836E-
 04 3
 7.56913988E-08-2.12407543E-11-8.56431436E+03 4.16902777E+01
 4
 C6H9r_R5_5 C 6 H 9 G 3E+02 1E+03 6E+02
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 06 3
 -2.71022592E-08 1.14081184E-11 2.33224843E+04 2.79718980E+01
 4
 C6H11O3r_3 C 6 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -2.06237512E+04 1.70587638E+01 3.99483848E+00 7.68564545E-02-7.11061649E-
 05 3
 4.42785349E-08-1.33898432E-11-2.06237512E+04 1.70587638E+01
 4
 C6H10O_Olef_6 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
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 11 2
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 04 3
 1.58554962E-07-5.49216310E-11 3.14376995E+03 3.32537457E+01
 4
 C6H11Or_Olef_33 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -5.18303491E+03 1.04161071E+01 4.83430344E+00 5.09226902E-02-7.77613973E-
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 cy(C*CC*CCJC) C 6 H 7 G 3E+02 1E+03 6E+02
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 9.89769162E-01 2.08229745E-02 7.09544963E-05-1.14720397E-07 4.92346711E-
 11 2
 2.37120517E+04 2.20321792E+01 9.89769162E-01 2.08229745E-02 7.09544963E-
 05 3
 -1.14720397E-07 4.92346711E-11 2.37120517E+04 2.20321792E+01
 4
 C6H7Or_Olef C 6 O 1 H 7 G 3E+02 1E+03 6E+02
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 1.07478277E+04 4.19935028E+01-4.12856454E+00 1.07855233E-01-1.53187139E-
 04 3
 1.17234521E-07-3.61469184E-11 1.07478277E+04 4.19935028E+01
 4
 C6H8O3_Olef_10 C 6 O 3 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -1.67506534E+04 4.65106574E+01-4.98333010E+00 1.45138433E-01-2.39458261E-
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 4
 cy(C*CC*CCC) C 6 H 8 G 3E+02 1E+03 6E+02
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 11 2
 1.10212970E+04 1.91308860E+01 1.72653190E+00 1.48876120E-02 9.48092301E-
 05 3
 -1.40833940E-07 5.88598730E-11 1.10212970E+04 1.91308860E+01
 4
 C6H10O2_Olef_10 C 6 O 2 H 10 G 3E+02 1E+03 6E+02
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 11 2
 -3.86270614E+03 3.26952285E+01-9.22987084E-01 9.82410059E-02-1.16441549E-
 04 3
 8.18876379E-08-2.49924172E-11-3.86270614E+03 3.26952285E+01
 4
 C6H8O_Olef_18 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -1.05372306E+04 4.02904848E+01-3.07159465E+00 9.03877582E-02-1.01411779E-
 04 3

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 4
 C6H9r_R5 C 6 H 9 G 3E+02 1E+03 6E+02
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 06 3
 -2.25698749E-08 8.85492052E-12 2.26036754E+04 2.83176513E+01
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 C6H11Or_Olef_52 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 -7.37772856E-02 8.20953409E-02-7.60739579E-05 3.87246545E-08-7.92197531E-
 12 2
 -4.09164906E+03 2.92848013E+01-7.37772856E-02 8.20953409E-02-7.60739579E-
 05 3
 3.87246545E-08-7.92197531E-12-4.09164906E+03 2.92848013E+01
 4
 C6H8O_Olef C 6 O 1 H 8 G 3E+02 1E+03 6E+02
 1
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 11 2
 7.56314364E+03 2.40527593E+00 4.33828091E+00 4.45222532E-02 8.54763832E-
 06 3
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 11 2
 7.75337560E+03 3.95864995E+01-3.11761848E+00 6.36384024E-02-1.72320343E-
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 C4H6O_Olef_1 C 4 O 1 H 6 G 3E+02 1E+03 6E+02
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 11 2
 -9.26965667E+03 4.60822795E+01-5.17940398E+00 8.11199405E-02-9.69327011E-
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 4
 C6H7Or_Olef_1 C 6 O 1 H 7 G 3E+02 1E+03 6E+02
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 11 2
 1.35855641E+04 3.09419273E+01-1.28080915E+00 9.73386177E-02-1.48817515E-
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 4
 C6H10O_Olef_4 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
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 11 2
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C6H9r_R5_1 C 6 H 9 G 3E+02 1E+03 6E+02
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 12 2
 1.52455893E+04 2.96019158E+01-1.10877088E+00 4.99289259E-02-1.37269628E-
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 C*cy(CCJC*CC) C 6 H 7 G 3E+02 1E+03 6E+02
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 2.56705107E+04 4.95661914E+01-5.60265480E+00 7.53828873E-02-6.51227472E-
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 2.57336068E-08-2.66191459E-12 2.56705107E+04 4.95661914E+01
 4
 C6H9r_R5_7 C 6 H 9 G 3E+02 1E+03 6E+02
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 11 2
 2.34656621E+04 3.65070996E+01-1.70183388E+00 4.18164423E-02 2.80258579E-
 05 3
 -6.77174314E-08 3.04521541E-11 2.34656621E+04 3.65070996E+01
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 11 2
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 04 3
 1.82778288E-07-6.45929517E-11 4.21850282E+03 3.00805766E+01
 4
 cy(CJCCCCC) C 6 H 11 G 3E+02 1E+03 6E+02
 1
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 11 2
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 04 3
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 4
 C6H9Or_Olef_2 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
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 11 2
 -1.49438210E+01 4.56685612E+00 6.12637201E+00 3.19718305E-02 1.59975008E-
 05 3
 -3.80384010E-08 1.61992647E-11-1.49438210E+01 4.56685612E+00
 4
 C6H8O_Olef_2 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 2.18898297E+00 6.70744260E-02-5.50809766E-05 2.09421218E-08-2.05614384E-
 12 2
 -3.93794474E+03-3.30561344E+00 2.18898297E+00 6.70744260E-02-5.50809766E-
 05 3
 2.09421218E-08-2.05614384E-12-3.93794474E+03-3.30561344E+00
 4
 cy(C*CCCC) C 5 H 8 G 3E+02 1E+03 6E+02
 1

-3.25550830E+00 4.57042848E-02 9.65396548E-07-3.40315995E-08 1.70883439E-
 11 2
 3.16828121E+03 4.02270550E+01-3.25550830E+00 4.57042848E-02 9.65396548E-
 07 3
 -3.40315995E-08 1.70883439E-11 3.16828121E+03 4.02270550E+01
 4
 C6H10O2_Olef_8 C 6 O 2 H 10 G 3E+02 1E+03 6E+02
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 1.62821718E+00 8.34453100E-02-8.76678352E-05 5.73170147E-08-1.71650987E-
 11 2
 -4.82577225E+03 2.03180054E+01 1.62821718E+00 8.34453100E-02-8.76678352E-
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 5.73170147E-08-1.71650987E-11-4.82577225E+03 2.03180054E+01
 4
 C6H9Or_Olef_6 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
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 11 2
 1.19361160E+03 6.23642782E+00 6.03327599E+00 3.42779635E-02 1.17027639E-
 05 3
 -3.50323181E-08 1.54565160E-11 1.19361160E+03 6.23642782E+00
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 C6H10O_Olef_11 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
 1
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 11 2
 -2.11601251E+04 3.22433801E+01-1.28551163E+00 8.95355663E-02-1.05471351E-
 04 3
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 C6H9r_R5_2 C 6 H 9 G 3E+02 1E+03 6E+02
 1
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 11 2
 2.27032521E+04 3.57366074E+01-1.24212857E+00 4.04679942E-02 1.26095096E-
 05 3
 -3.65289075E-08 1.47172189E-11 2.27032521E+04 3.57366074E+01
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 11 2
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 04 3
 8.66513518E-08-2.37435336E-11 1.91210859E+04 4.13997903E+01
 4
 C5H7Or_Olef C 5 O 1 H 7 G 3E+02 1E+03 6E+02
 1
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 12 2
 4.32359751E+03 1.18163029E+01 4.39743041E+00 3.22420869E-02-1.65896601E-
 06 3
 -1.74549302E-08 8.70250462E-12 4.32359751E+03 1.18163029E+01
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 cy(C*CCJCCC) C 6 H 9 G 3E+02 1E+03 6E+02
 1
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 12 2

1.46615475E+04 2.97419048E+01-1.75159018E+00 5.51905093E-02-1.41103474E-
 05 3
 -1.65560601E-08 9.15307897E-12 1.46615475E+04 2.97419048E+01
 4
 C6H11Or_Olef_22 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 1.42843879E+00 6.33399588E-02-2.03772004E-05-2.28360444E-08 1.53587988E-
 11 2
 -7.14851998E+03 2.24949250E+01 1.42843879E+00 6.33399588E-02-2.03772004E-
 05 3
 -2.28360444E-08 1.53587988E-11-7.14851998E+03 2.24949250E+01
 4
 C6H11Or_Olef_1 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 4.43698730E+00 4.95401319E-02-1.46515292E-06-3.39402303E-08 1.78130289E-
 11 2
 -3.25919345E+03 1.10634346E+01 4.43698730E+00 4.95401319E-02-1.46515292E-
 06 3
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 4
 Ccy (CJC*CC*C) C 6 H 7 G 3E+02 1E+03 6E+02
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 -2.89065384E+00 5.80727701E-02-2.90826750E-05-7.90540076E-09 9.03196891E-
 12 2
 2.53738459E+04 3.93062817E+01-2.89065384E+00 5.80727701E-02-2.90826750E-
 05 3
 -7.90540076E-09 9.03196891E-12 2.53738459E+04 3.93062817E+01
 4
 C6H11Or_Olef_3 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
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 11 2
 -1.35095797E+04 1.14042725E+01 4.12528397E+00 4.42489537E-02 1.46769634E-
 05 3
 -4.96182647E-08 2.30287825E-11-1.35095797E+04 1.14042725E+01
 4
 C6H8O_Olef_15 C 6 O 1 H 8 G 3E+02 1E+03 6E+02
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 11 2
 -5.72657793E+03 3.06387022E+01-1.02726094E+00 8.58446500E-02-1.09292213E-
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 4
 C*cy (CCC*CC) C 6 H 8 G 3E+02 1E+03 6E+02
 1
 1.64498967E-01 4.33524906E-02-9.06382279E-06-1.06521290E-08 4.86459018E-
 12 2
 1.43744093E+04 2.36485599E+01 1.64498967E-01 4.33524906E-02-9.06382279E-
 06 3
 -1.06521290E-08 4.86459018E-12 1.43744093E+04 2.36485599E+01
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 C4H7Or_Olef_1 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
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 5.02838016E-01 5.01581602E-02-3.10817978E-05-7.98113218E-10 5.91960889E-
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 C6H10_Olef_1 C 6 H 10 G 3E+02 1E+03 6E+02
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 11 2
 5.06504719E+03 2.55440807E+01 6.40068295E-01 4.66256718E-02 1.52144648E-
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 4
 C6H8O3_Olef_4 C 6 O 3 H 8 G 3E+02 1E+03 6E+02
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 12 2
 -1.45346556E+04 1.39069321E+01 3.89416427E+00 6.79499966E-02-5.04093668E-
 05 3
 1.73585769E-08-2.24722794E-12-1.45346556E+04 1.39069321E+01
 4
 C4H7Or_Olef_4 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 2.91175815E+00 3.90982474E-02-2.33862589E-05 3.96911638E-09 1.40891075E-
 12 2
 8.93036278E+03 1.59481656E+01 2.91175815E+00 3.90982474E-02-2.33862589E-
 05 3
 3.96911638E-09 1.40891075E-12 8.93036278E+03 1.59481656E+01
 4
 C6H9Or_Olef_3 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
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 2.30894779E+00 5.42314461E-02-2.91942662E-05 1.78747184E-09 3.21434593E-
 12 2
 1.02100788E+03 2.13457675E+01 2.30894779E+00 5.42314461E-02-2.91942662E-
 05 3
 1.78747184E-09 3.21434593E-12 1.02100788E+03 2.13457675E+01
 4
 Ccy(C*CCC*C) C 6 H 8 G 3E+02 1E+03 6E+02
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 -2.58870532E+00 5.20170248E-02-6.52041052E-06-3.13902857E-08 1.74194278E-
 11 2
 1.06006079E+04 3.79252620E+01-2.58870532E+00 5.20170248E-02-6.52041052E-
 06 3
 -3.13902857E-08 1.74194278E-11 1.06006079E+04 3.79252620E+01
 4
 CC*CCCJ C 5 H 9 G 3E+02 1E+03 6E+02
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 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
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 11 2
 9.38202914E+03 2.38898373E+01 7.57752522E-02 9.70957113E-02-1.19831860E-
 04 3
 8.66404185E-08-2.69636226E-11 9.38202914E+03 2.38898373E+01
 4

C*CCCCJCOH C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 -3.26977569E+03 1.04893707E+01 5.42391062E+00 4.06474704E-02 1.40829584E-
 05 3
 -4.38511969E-08 1.98000458E-11-3.26977569E+03 1.04893707E+01
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 C6H11Or_Olef_54 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 05 3
 2.54760165E-08-4.16061532E-12-5.61234329E+03 2.58326720E+01
 4
 C6H11Or_Olef_25 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
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 2.93027975E+00 4.93877756E-02 9.98070754E-06-4.96804581E-08 2.40033906E-
 11 2
 -8.65087053E+03 1.66663270E+01 2.93027975E+00 4.93877756E-02 9.98070754E-
 06 3
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 4
 C6H9O2r_Olef C 6 O 2 H 9 G 3E+02 1E+03 6E+02
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 11 2
 1.52425783E+04 1.42086215E+01 3.86634260E+00 6.79606563E-02-7.50240202E-
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 4
 C3H5Or_Olef_2 C 3 O 1 H 5 G 3E+02 1E+03 6E+02
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 13 2
 1.25544263E+04 1.83172066E+00 5.11009153E+00 2.31498546E-02-1.46256674E-
 05 3
 4.92418304E-09-5.51487062E-13 1.25544263E+04 1.83172066E+00
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 CJcy(CCCCC) C 6 H 11 G 3E+02 1E+03 6E+02
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 11 2
 1.01558070E+04 3.74241919E+01-1.69292471E+00 5.02194893E-02 1.64863893E-
 05 3
 -5.68204725E-08 2.63807655E-11 1.01558070E+04 3.74241919E+01
 4
 C6H11O3r_5 C 6 O 3 H 11 G 3E+02 1E+03 6E+02
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 11 2
 -2.06237512E+04 1.70587638E+01 3.99483848E+00 7.68564545E-02-7.11061649E-
 05 3
 4.42785349E-08-1.33898432E-11-2.06237512E+04 1.70587638E+01
 4
 C6H9Or_Olef_22 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
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 11 2
 1.11068457E+04 2.17473846E+01 1.14773154E+00 6.16146920E-02-2.70694537E-
 05 3
 -1.20286957E-08 1.04772043E-11 1.11068457E+04 2.17473846E+01
 4
 C6H11r_Olef_4 C 6 H 11 G 3E+02 1E+03 6E+02
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 1.25986000E+00 5.66800000E-02-2.95700000E-05 4.90499997E-09 5.99100008E-
 13 2
 1.64200000E+04 2.49100000E+01 1.25986000E+00 5.66800000E-02-2.95700000E-
 05 3
 4.90499997E-09 5.99100008E-13 1.64200000E+04 2.49100000E+01
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 CJ*CCC*C C 5 H 7 G100.000 5000.000 2054.51
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 13 2
 6.38123815E+04 2.45431012E+02 9.71313023E-01 4.37224571E-02-2.95961711E-
 05 3
 1.18941145E-08-2.42217143E-12 4.05334717E+04 2.42924004E+01
 4
 C6H9Or_Olef_12 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
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 12 2
 1.38674004E+04 1.56141569E+01 3.26691164E+00 5.35329527E-02-2.69467158E-
 05 3
 2.23417349E-10 3.29618012E-12 1.38674004E+04 1.56141569E+01
 4
 C3H5Or_Olef C 3 O 1 H 5 G 3E+02 1E+03 6E+02
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 -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
 C6H11Or_Olef_37 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 4.92739946E+00 4.86165571E-02-3.48140280E-06-2.85935919E-08 1.49698722E-
 11 2
 -6.39159033E+03 8.74653543E+00 4.92739946E+00 4.86165571E-02-3.48140280E-
 06 3
 -2.85935919E-08 1.49698722E-11-6.39159033E+03 8.74653543E+00
 4
 C6H10O_Olef_2 C 6 O 1 H 10 G 3E+02 1E+03 6E+02
 1
 -3.88993922E-01 8.12559265E-02-8.89265562E-05 6.36948867E-08-2.01447616E-
 11 2
 -2.43415968E+04 3.02726277E+01-3.88993922E-01 8.12559265E-02-8.89265562E-
 05 3
 6.36948867E-08-2.01447616E-11-2.43415968E+04 3.02726277E+01
 4
 cy(C*CCCJCC) C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -1.30647405E+00 5.18258104E-02-1.11305087E-05-1.65053204E-08 8.46589756E-
 12 2

2.20012900E+04 3.15272563E+01-1.30647405E+00 5.18258104E-02-1.11305087E-05 3
 -1.65053204E-08 8.46589756E-12 2.20012900E+04 3.15272563E+01
 4
 C6H11Or_Olef_31 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 3.45093833E+00 4.86346550E-02 3.59495746E-06-3.89732071E-08 1.93766434E-11 2
 -4.53625057E+03 1.72881986E+01 3.45093833E+00 4.86346550E-02 3.59495746E-06 3
 -3.89732071E-08 1.93766434E-11-4.53625057E+03 1.72881986E+01
 4
 CJcy(CC*CCC) C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -1.13259641E+00 5.15978779E-02-1.35082748E-05-1.38536212E-08 7.64675836E-12 2
 2.48431785E+04 3.14240272E+01-1.13259641E+00 5.15978779E-02-1.35082748E-05 3
 -1.38536212E-08 7.64675836E-12 2.48431785E+04 3.14240272E+01
 4
 C5H8O_Olef_6 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 8.06413059E-01 5.38838202E-02-2.35045899E-05-1.32100953E-08 1.10672725E-11 2
 -1.26187771E+04 2.37595650E+01 8.06413059E-01 5.38838202E-02-2.35045899E-05 3
 -1.32100953E-08 1.10672725E-11-1.26187771E+04 2.37595650E+01
 4
 C6H11Or_Olef_28 C 6 O 1 H 11 G 3E+02 1E+03 6E+02
 1
 2.34268021E+00 5.66965575E-02-7.57927548E-06-3.30785994E-08 1.83774100E-11 2
 -7.46065879E+03 2.07123675E+01 2.34268021E+00 5.66965575E-02-7.57927548E-06 3
 -3.30785994E-08 1.83774100E-11-7.46065879E+03 2.07123675E+01
 4
 C5H8O_Olef_3 C 5 O 1 H 8 G 3E+02 1E+03 6E+02
 1
 -3.45046238E+00 8.08496842E-02-7.92762343E-05 3.70615536E-08-5.73875626E-12 2
 -1.36081980E+04 3.99314450E+01-3.45046238E+00 8.08496842E-02-7.92762343E-05 3
 3.70615536E-08-5.73875626E-12-1.36081980E+04 3.99314450E+01
 4
 C6H8O3_Olef_3 C 6 O 3 H 8 G 3E+02 1E+03 6E+02
 1
 1.29910703E+00 1.06940873E-01-1.68642567E-04 1.51024474E-07-5.37396228E-11 2
 -1.75251476E+04 2.29256517E+01 1.29910703E+00 1.06940873E-01-1.68642567E-04 3
 1.51024474E-07-5.37396228E-11-1.75251476E+04 2.29256517E+01
 4
 C6H11O3r_1 C 6 H 11 O 3 G100.000 5000.000 655.09
 1
 8.04560515E+00 5.79854417E-02-2.85144545E-05 5.30482805E-09-3.56040184E-13 2
 -1.38685985E+04-3.24561720E+00 4.28020797E-01 7.81375139E-02-1.42962775E-05 3

-7.05938505E-08 5.20523445E-11-1.23049316E+04 3.45999148E+01
 4
 C6H9Or_Olef_5 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 -1.53905984E+00 1.01029534E-01-1.44996653E-04 1.19597135E-07-3.96686330E-
 11 2
 -1.84798309E+03 3.25466051E+01-1.53905984E+00 1.01029534E-01-1.44996653E-
 04 3
 1.19597135E-07-3.96686330E-11-1.84798309E+03 3.25466051E+01
 4
 C*CCJC*CC C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -2.39267611E-01 4.31154844E-02 2.78574260E-05-7.22799949E-08 3.32716149E-
 11 2
 1.45763853E+04 2.60125973E+01-2.39267611E-01 4.31154844E-02 2.78574260E-
 05 3
 -7.22799949E-08 3.32716149E-11 1.45763853E+04 2.60125973E+01
 4
 fulvene C 6 H 6 G 3E+02 1E+03 6E+02
 1
 -4.52117585E+00 6.48445984E-02-4.82396311E-05 1.16888805E-08 1.79226753E-
 12 2
 2.53908694E+04 4.37971407E+01-4.52117585E+00 6.48445984E-02-4.82396311E-
 05 3
 1.16888805E-08 1.79226753E-12 2.53908694E+04 4.37971407E+01
 4
 C6H11O3r_7 C 6 O 3 H 11 G 3E+02 1E+03 6E+02
 1
 6.87394462E+00 5.77256113E-02-2.89391704E-05 8.64252044E-09-2.91201509E-
 12 2
 -1.20553869E+04 5.12496019E+00 6.87394462E+00 5.77256113E-02-2.89391704E-
 05 3
 8.64252044E-09-2.91201509E-12-1.20553869E+04 5.12496019E+00
 4
 C*CCCC(*O)C C 6 O 1 H 10 G 3E+02 1E+03 6E+02
 1
 6.29534225E+00 2.62888139E-02 4.34486038E-05-6.99436545E-08 2.82544441E-
 11 2
 -2.17455290E+04 4.33701110E+00 6.29534225E+00 2.62888139E-02 4.34486038E-
 05 3
 -6.99436545E-08 2.82544441E-11-2.17455290E+04 4.33701110E+00
 4
 C4H6O_Olef C 4 O 1 H 6 G 3E+02 1E+03 6E+02
 1
 -1.66246256E+00 5.46510568E-02-3.40122495E-05-4.31562560E-09 8.66884600E-
 12 2
 -1.05899350E+04 3.23228275E+01-1.66246256E+00 5.46510568E-02-3.40122495E-
 05 3
 -4.31562560E-09 8.66884600E-12-1.05899350E+04 3.23228275E+01
 4
 C4H7Or_Olef_5 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 -9.06282037E-01 6.66074092E-02-8.24838184E-05 5.77565027E-08-1.66184164E-
 11 2
 1.66637569E+03 2.88142212E+01-9.06282037E-01 6.66074092E-02-8.24838184E-
 05 3
 5.77565027E-08-1.66184164E-11 1.66637569E+03 2.88142212E+01
 4

C4H7Or_Olef_3 C 4 O 1 H 7 G 3E+02 1E+03 6E+02
 1
 6.50500474E-01 6.11082908E-02-7.33521809E-05 5.00641063E-08-1.40313287E-
 11 2
 7.55875976E+03 2.15577892E+01 6.50500474E-01 6.11082908E-02-7.33521809E-
 05 3
 5.00641063E-08-1.40313287E-11 7.55875976E+03 2.15577892E+01
 4
 C6H9O2r_Olef_11 C 6 O 2 H 9 G 3E+02 1E+03 6E+02
 1
 1.01858721E+00 7.84772713E-02-7.93936440E-05 4.96044761E-08-1.43326588E-
 11 2
 1.24048418E+04 2.41615847E+01 1.01858721E+00 7.84772713E-02-7.93936440E-
 05 3
 4.96044761E-08-1.43326588E-11 1.24048418E+04 2.41615847E+01
 4
 C*CCCCCJ C 6 H 11 G 3E+02 1E+03 6E+02
 1
 1.15861999E-01 6.21400000E-02-3.75200000E-05 9.75399999E-09-4.75600001E-
 13 2
 1.77800000E+04 3.11200000E+01 1.15861999E-01 6.21400000E-02-3.75200000E-
 05 3
 9.75399999E-09-4.75600001E-13 1.77800000E+04 3.11200000E+01
 4
 C6H9Or_Olef_9 C 6 O 1 H 9 G 3E+02 1E+03 6E+02
 1
 5.24431856E+00 3.51661589E-02 2.08415263E-05-4.85705325E-08 2.07948194E-
 11 2
 1.18296014E+04 6.00463780E+00 5.24431856E+00 3.51661589E-02 2.08415263E-
 05 3
 -4.85705325E-08 2.07948194E-11 1.18296014E+04 6.00463780E+00
 4
 C6H10O2_Olef_5 C 6 O 2 H 10 G 3E+02 1E+03 6E+02
 1
 3.90217523E+00 6.93575971E-02-6.42836828E-05 4.13766551E-08-1.32257745E-
 11 2
 -3.06276868E+03 1.31327462E+01 3.90217523E+00 6.93575971E-02-6.42836828E-
 05 3
 4.13766551E-08-1.32257745E-11-3.06276868E+03 1.31327462E+01
 4
 C6H9Or_Olef_13 C 6 H 9 O 1 G100.000 5000.000 903.75
 1
 8.00722176E+00 4.04651586E-02-1.84995805E-05 3.43469799E-09-2.34005796E-
 13 2
 1.01859144E+04-9.31085735E+00 1.21883964E+00 5.35440063E-02-1.20469952E-
 05 3
 -2.20980035E-08 1.25752663E-11 1.21057987E+04 2.65855432E+01
 4
 cy(C*CCCC) C 6 H 10 G 3E+02 1E+03 6E+02
 1
 -2.06482463E+00 4.27134700E-02 3.32453709E-05-7.32560661E-08 3.21239676E-
 11 2
 -1.49550613E+03 3.47780171E+01-2.06482463E+00 4.27134700E-02 3.32453709E-
 05 3
 -7.32560661E-08 3.21239676E-11-1.49550613E+03 3.47780171E+01
 4
 cy(CJC*CcyCCC) C 6 H 7 G250.000 5000.000 995.00
 1

1.51800569E+01 1.73086061E-02-5.43127401E-06 7.91962369E-10-4.39096961E-
14 2
2.78279003E+04-6.02528765E+01 2.87077864E+00 2.42200781E-03 1.14044401E-
04 3
-1.44267266E-07 5.27355286E-11 3.34641723E+04 1.50835830E+01
4
C*CCCC (C) CJ C 7 H 13 G 3E+02 1E+03 6E+02
1
3.44743527E+00 5.49296012E-02 1.68605163E-06-3.92428872E-08 1.95590240E-
11 2
1.35944401E+04 1.33516702E+01 3.44743527E+00 5.49296012E-02 1.68605163E-
06 3
-3.92428872E-08 1.95590240E-11 1.35944401E+04 1.33516702E+01
4
C*CCCCJCCC*C C 9 H 15 G 3E+02 1E+03 6E+02
1
7.66970833E+00 4.06497161E-02 6.00050946E-05-1.01819796E-07 4.21366479E-
11 2
2.25156525E+04 4.02050748E+00 7.66970833E+00 4.06497161E-02 6.00050946E-
05 3
-1.01819796E-07 4.21366479E-11 2.25156525E+04 4.02050748E+00
4
C*CCCC (CJ) CC*C C 9 H 15 G 3E+02 1E+03 6E+02
1
4.24543520E+00 6.73967109E-02 1.72237648E-06-4.84500651E-08 2.42367876E-
11 2
2.31867588E+04 1.56742327E+01 4.24543520E+00 6.73967109E-02 1.72237648E-
06 3
-4.84500651E-08 2.42367876E-11 2.31867588E+04 1.56742327E+01
4
CC*CCJC C 5 H 9 G 3E+02 1E+03 6E+02
1
1.49390000E+00 4.01700000E-02-9.71399997E-06-7.85100002E-09 3.78000000E-
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
1
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
C*CCJCC (C) CC*C C 9 H 15 G 3E+02 1E+03 6E+02
1
3.61496885E+00 6.50952033E-02 1.04644971E-05-5.70495585E-08 2.70910686E-
11 2
1.30352427E+04 1.66444464E+01 3.61496885E+00 6.50952033E-02 1.04644971E-
05 3
-5.70495585E-08 2.70910686E-11 1.30352427E+04 1.66444464E+01
4
CC*CCC 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
C*CCCC C 5 H 10 G 3E+02 1E+03 6E+02
1
3.59709404E+00 2.81126994E-02 2.86626078E-05-5.29107130E-08 2.20767194E-
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
cy(C*CCCJC) C 5 H 7 G 3E+02 1E+03 6E+02
1
1.19451240E-01 2.51329647E-02 2.36879897E-05-3.91127583E-08 1.41772047E-
11 2
2.72641880E+04 2.69580514E+01 1.19451240E-01 2.51329647E-02 2.36879897E-
05 3
-3.91127583E-08 1.41772047E-11 2.72641880E+04 2.69580514E+01
4
C6H9-A C 6 H 9 G 3E+02 1E+03 6E+02
1
1.21662000E+00 5.34500000E-02-3.04800000E-05 6.24799999E-09 2.97799999E-
13 2
2.43200000E+04 2.32200000E+01 1.21662000E+00 5.34500000E-02-3.04800000E-
05 3
6.24799999E-09 2.97799999E-13 2.43200000E+04 2.32200000E+01
4
C*CCCC (CJ) CC C 8 H 15 G 3E+02 1E+03 6E+02
1
5.08328085E+00 5.69654778E-02 1.50477815E-05-5.68202750E-08 2.63130353E-
11 2
1.04644542E+04 8.46494237E+00 5.08328085E+00 5.69654778E-02 1.50477815E-
05 3
-5.68202750E-08 2.63130353E-11 1.04644542E+04 8.46494237E+00
4
C*CCCCJCCC C 8 H 15 G 3E+02 1E+03 6E+02
1
8.50755398E+00 3.02184830E-02 7.33304996E-05-1.10190006E-07 4.42128956E-
11 2
9.79334795E+03-1.80248850E+00 8.50755398E+00 3.02184830E-02 7.33304996E-
05 3
-1.10190006E-07 4.42128956E-11 9.79334795E+03-1.80248850E+00
4
C*CCJCC (C) CC C 8 H 15 G 3E+02 1E+03 6E+02
1
4.45281449E+00 5.46639702E-02 2.37899022E-05-6.54197683E-08 2.91673163E-
11 2
3.12938147E+02 9.43515603E+00 4.45281449E+00 5.46639702E-02 2.37899022E-
05 3
-6.54197683E-08 2.91673163E-11 3.12938147E+02 9.43515603E+00
4
C*CC (C) CCJC*C C 8 H 13 G 3E+02 1E+03 6E+02
1
4.45153944E+00 5.12370494E-02 2.19181970E-05-6.31307532E-08 2.86444029E-
11 2
1.59456094E+04 1.03468973E+01 4.45153944E+00 5.12370494E-02 2.19181970E-
05 3

-6.31307532E-08 2.86444029E-11 1.59456094E+04 1.03468973E+01
 4
 C*CCCJCCC*C C 8 H 13 G 3E+02 1E+03 6E+02
 1
 6.18961181E+00 3.97016302E-02 4.08033852E-05-7.60660418E-08 3.18543387E-
 11 2
 2.52872814E+04 8.48595541E+00 6.18961181E+00 3.97016302E-02 4.08033852E-
 05 3
 -7.60660418E-08 3.18543387E-11 2.52872814E+04 8.48595541E+00
 4
 C*CC (CJ) CCC*C C 8 H 13 G 3E+02 1E+03 6E+02
 1
 3.79622210E+00 5.91280178E-02 3.51063694E-06-4.68252926E-08 2.34531128E-
 11 2
 2.60146015E+04 1.54621902E+01 3.79622210E+00 5.91280178E-02 3.51063694E-
 06 3
 -4.68252926E-08 2.34531128E-11 2.60146015E+04 1.54621902E+01
 4
 C*CCJCC (C) C C 7 H 13 G 3E+02 1E+03 6E+02
 1
 2.81696891E+00 5.26280935E-02 1.04281722E-05-4.78423805E-08 2.24133049E-
 11 2
 3.44292406E+03 1.43218839E+01 2.81696891E+00 5.26280935E-02 1.04281722E-
 05 3
 -4.78423805E-08 2.24133049E-11 3.44292406E+03 1.43218839E+01
 4
 C*CCCC*CC C 7 H 12 G 3E+02 1E+03 6E+02
 1
 4.48819000E+00 3.82736761E-02 3.29936696E-05-6.51239740E-08 2.74972319E-
 11 2
 3.48706055E+03 1.21614062E+01 4.48819000E+00 3.82736761E-02 3.29936696E-
 05 3
 -6.51239740E-08 2.74972319E-11 3.48706055E+03 1.21614062E+01
 4
 C*CC (C) CC*C C 7 H 12 G 3E+02 1E+03 6E+02
 1
 3.00904170E+00 5.10566624E-02 8.49884626E-06-4.61257798E-08 2.21146172E-
 11 2
 3.90224182E+03 1.66619363E+01 3.00904170E+00 5.10566624E-02 8.49884626E-
 06 3
 -4.61257798E-08 2.21146172E-11 3.90224182E+03 1.66619363E+01
 4
 C*C (C) CCC*C C 7 H 12 G 3E+02 1E+03 6E+02
 1
 2.47064593E+00 5.49725457E-02-5.83266496E-06-2.79976198E-08 1.46781875E-
 11 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
 CJ*CCCC*C C 6 H 9 G 3E+02 1E+03 6E+02
 1
 -5.89279806E-01 6.49227420E-02-5.76701426E-05 3.28250096E-08-9.04457697E-
 12 2
 3.82598492E+04 3.27664193E+01-5.89279806E-01 6.49227420E-02-5.76701426E-
 05 3
 3.28250096E-08-9.04457697E-12 3.82598492E+04 3.27664193E+01
 4

C*CJCCC*C C 6 H 9 G 3E+02 1E+03 6E+02
 1
 4.48582748E-01 5.64074288E-02-3.74503021E-05 1.31522035E-08-2.16462986E-
 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
 C(*O)COJ C 2 H 3 O 2 G100.000 5000.000 894.97
 1
 7.25459482E+00 1.13752940E-02-4.73840666E-06 9.21761286E-10-6.75104790E-
 14 2
 -1.22403679E+04-1.02827390E+01 2.88717886E+00 1.35907195E-02 2.05510594E-
 05 3
 -3.95204763E-08 1.72643893E-11-1.07656058E+04 1.41746306E+01
 4
 Ccy(CC*(C)C*(C) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -7.57242825E-01 6.42633642E-02-2.16485897E-05-2.19947320E-08 1.54770311E-
 11 2
 7.74064481E+03 2.77355048E+01-7.57242825E-01 6.42633642E-02-2.16485897E-
 05 3
 -2.19947320E-08 1.54770311E-11 7.74064481E+03 2.77355048E+01
 4
 C7H10_R5_3 C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -2.89466950E+00 8.01030084E-02-9.65105076E-05 8.36340461E-08-3.07766783E-
 11 2
 8.37425895E+03 3.95538250E+01-2.89466950E+00 8.01030084E-02-9.65105076E-
 05 3
 8.36340461E-08-3.07766783E-11 8.37425895E+03 3.95538250E+01
 4
 C7H11r_Olef_15 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 3.51445872E-01 6.30507055E-02-5.95506484E-06-4.02474480E-08 2.18579708E-
 11 2
 1.49333961E+04 2.55157505E+01 3.51445872E-01 6.30507055E-02-5.95506484E-
 06 3
 -4.02474480E-08 2.18579708E-11 1.49333961E+04 2.55157505E+01
 4
 C7H11r_R5_75 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.40686582E+00 5.98677976E-02-1.08485357E-05-2.10706079E-08 1.05413669E-
 11 2
 1.30716330E+04 3.24820874E+01-1.40686582E+00 5.98677976E-02-1.08485357E-
 05 3
 -2.10706079E-08 1.05413669E-11 1.30716330E+04 3.24820874E+01
 4
 C7H11r_R5_51 C 7 H 11 G 3E+02 2E+03 1E+03
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 -3.12129481E-02 5.40702132E-02 2.58586322E-06-3.68618096E-08 1.70495937E-
 11 2
 1.97563596E+04 2.56424773E+01-3.12129481E-02 5.40702132E-02 2.58586322E-
 06 3
 -3.68618096E-08 1.70495937E-11 1.97563596E+04 2.56424773E+01
 4
 C*CCJCC*CC C 7 H 11 G 3E+02 2E+03 1E+03
 1

7.02638516E+00 2.43305325E-02 5.59143892E-05-8.45740025E-08 3.38910593E-
 11 2
 1.82406352E+04-2.56221693E+00 7.02638516E+00 2.43305325E-02 5.59143892E-
 05 3
 -8.45740025E-08 3.38910593E-11 1.82406352E+04-2.56221693E+00
 4
 Ccy(C*C(C)C*CC) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 2.03483659E+00 4.78565022E-02 1.01498616E-05-4.87853115E-08 2.38999518E-
 11 2
 6.28693036E+03 1.57940232E+01 2.03483659E+00 4.78565022E-02 1.01498616E-
 05 3
 -4.87853115E-08 2.38999518E-11 6.28693036E+03 1.57940232E+01
 4
 C7H9r_R5_3 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.18260185E+00 6.60462692E-02-5.18986906E-05 2.48730812E-08-4.92714350E-
 12 2
 3.36176395E+04 3.95674689E+01-2.18260185E+00 6.60462692E-02-5.18986906E-
 05 3
 2.48730812E-08-4.92714350E-12 3.36176395E+04 3.95674689E+01
 4
 C7H11r_Olef_5 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 4.09373475E+00 5.16043041E-02-8.50776834E-06-2.34825659E-08 1.30128417E-
 11 2
 2.77304118E+04 9.11057047E+00 4.09373475E+00 5.16043041E-02-8.50776834E-
 06 3
 -2.34825659E-08 1.30128417E-11 2.77304118E+04 9.11057047E+00
 4
 C*Ccy(CCC*CC) C 7 H 10 G 3E+02 2E+03 1E+03
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 -1.12171320E+00 5.59904536E-02-8.48325901E-06-2.23600170E-08 1.09854028E-
 11 2
 1.23224379E+04 3.31526942E+01-1.12171320E+00 5.59904536E-02-8.48325901E-
 06 3
 -2.23600170E-08 1.09854028E-11 1.23224379E+04 3.31526942E+01
 4
 C7H11r_R5_55 C 7 H 11 G 3E+02 2E+03 1E+03
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 -1.47620812E+00 6.16127017E-02-1.89835425E-05-1.05435298E-08 6.24157762E-
 12 2
 1.26108124E+04 3.45941222E+01-1.47620812E+00 6.16127017E-02-1.89835425E-
 05 3
 -1.05435298E-08 6.24157762E-12 1.26108124E+04 3.45941222E+01
 4
 CCJcyCC*CC*C C 7 H 9 G 3E+02 2E+03 1E+03
 1
 3.69285550E-01 4.42463437E-02 4.22631794E-05-9.75760907E-08 4.51257206E-
 11 2
 3.30740906E+04 2.43298786E+01 3.69285550E-01 4.42463437E-02 4.22631794E-
 05 3
 -9.75760907E-08 4.51257206E-11 3.30740906E+04 2.43298786E+01
 4
 C7H11r_R5_3 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.36218926E+00 6.18821453E-02-2.07164394E-06-4.61058824E-08 2.49449842E-
 11 2

2.16862534E+04 3.42437114E+01-1.36218926E+00 6.18821453E-02-2.07164394E-
 06 3
 -4.61058824E-08 2.49449842E-11 2.16862534E+04 3.42437114E+01
 4
 CC*CC*CCJC C 7 H 11 G 3E+02 2E+03 1E+03
 1
 2.36887541E+00 4.63527839E-02 3.28690656E-05-7.73716945E-08 3.46762874E-
 11 2
 1.52553491E+04 1.65016488E+01 2.36887541E+00 4.63527839E-02 3.28690656E-
 05 3
 -7.73716945E-08 3.46762874E-11 1.52553491E+04 1.65016488E+01
 4
 Ccy(C*CCCJC*C) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.16404284E+00 5.85479087E-02-6.62018094E-06-3.48057431E-08 1.87983183E-
 11 2
 1.76279334E+04 3.64476749E+01-2.16404284E+00 5.85479087E-02-6.62018094E-
 06 3
 -3.48057431E-08 1.87983183E-11 1.76279334E+04 3.64476749E+01
 4
 Ccy(CCJC*CC*C) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -3.46415936E+00 6.45891460E-02-1.73015067E-05-2.63901563E-08 1.62928176E-
 11 2
 1.86814054E+04 4.18805461E+01-3.46415936E+00 6.45891460E-02-1.73015067E-
 05 3
 -2.63901563E-08 1.62928176E-11 1.86814054E+04 4.18805461E+01
 4
 C7H9r_Olef C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.78592084E+00 6.17055500E-02-1.11255003E-05-3.24966448E-08 1.84990355E-
 11 2
 2.34551385E+04 3.83794211E+01-2.78592084E+00 6.17055500E-02-1.11255003E-
 05 3
 -3.24966448E-08 1.84990355E-11 2.34551385E+04 3.83794211E+01
 4
 C7H9r_R5_15 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 2.52121376E+00 3.69049550E-02 2.97389265E-05-6.46202301E-08 2.86517282E-
 11 2
 2.22040260E+04 1.48767259E+01 2.52121376E+00 3.69049550E-02 2.97389265E-
 05 3
 -6.46202301E-08 2.86517282E-11 2.22040260E+04 1.48767259E+01
 4
 C7H11r_Olef_9 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 3.89873863E+00 4.88027001E-02-4.17086175E-07-2.78134954E-08 1.34271466E-
 11 2
 1.31646538E+04 9.79479844E+00 3.89873863E+00 4.88027001E-02-4.17086175E-
 07 3
 -2.78134954E-08 1.34271466E-11 1.31646538E+04 9.79479844E+00
 4
 C7H11r_R5_60 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -4.13837951E-01 5.90736032E-02-1.75844824E-05-1.05587764E-08 6.08548867E-
 12 2
 1.86609123E+04 2.79433676E+01-4.13837951E-01 5.90736032E-02-1.75844824E-
 05 3

-1.05587764E-08 6.08548867E-12 1.86609123E+04 2.79433676E+01
 4
 C*CCC*CCJC C 7 H 11 G 3E+02 2E+03 1E+03
 1
 4.20150760E+00 3.87221211E-02 2.87549211E-05-6.15419828E-08 2.65287514E-
 11 2
 1.98678415E+04 1.19963958E+01 4.20150760E+00 3.87221211E-02 2.87549211E-
 05 3
 -6.15419828E-08 2.65287514E-11 1.98678415E+04 1.19963958E+01
 4
 CC*cy(CCJC*CC) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.32818908E+00 6.56962410E-02-4.03115324E-05 1.50127480E-08-3.61417492E-
 12 2
 2.32894550E+04 3.77188058E+01-2.32818908E+00 6.56962410E-02-4.03115324E-
 05 3
 1.50127480E-08-3.61417492E-12 2.32894550E+04 3.77188058E+01
 4
 C7H11r_R5_27 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -3.35502881E+00 7.59285745E-02-4.51594973E-05 8.21921807E-09 1.45347556E-
 12 2
 2.11382376E+04 4.05500062E+01-3.35502881E+00 7.59285745E-02-4.51594973E-
 05 3
 8.21921807E-09 1.45347556E-12 2.11382376E+04 4.05500062E+01
 4
 C7H11r_Olef_3 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 9.23109010E-01 5.72495632E-02-1.06876661E-05-2.42368959E-08 1.36035573E-
 11 2
 9.85095116E+03 2.21008308E+01 9.23109010E-01 5.72495632E-02-1.06876661E-
 05 3
 -2.42368959E-08 1.36035573E-11 9.85095116E+03 2.21008308E+01
 4
 Ccy(C*CCC*CC) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 6.22207794E+00 3.59505278E-02 2.27081982E-05-5.09738124E-08 2.19235739E-
 11 2
 5.91687430E+03-1.78066674E+01 6.22207794E+00 3.59505278E-02 2.27081982E-
 05 3
 -5.09738124E-08 2.19235739E-11 5.91687430E+03-1.78066674E+01
 4
 Ccy(C*CCCC*C) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -1.05932624E+00 4.93669320E-02 2.06637643E-05-6.19598799E-08 2.83652171E-
 11 2
 6.27786382E+03 3.11241838E+01-1.05932624E+00 4.93669320E-02 2.06637643E-
 05 3
 -6.19598799E-08 2.83652171E-11 6.27786382E+03 3.11241838E+01
 4
 C7H11r_R5_17 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.06931810E+00 7.03394311E-02-3.54946066E-05 5.13688314E-10 3.79035209E-
 12 2
 2.12207569E+04 3.44648450E+01-2.06931810E+00 7.03394311E-02-3.54946066E-
 05 3
 5.13688314E-10 3.79035209E-12 2.12207569E+04 3.44648450E+01
 4

Ccy(CC*CCCCJ) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.21236097E+00 6.32471589E-02-1.21281973E-05-2.62654724E-08 1.41075399E-
 11 2
 1.84352403E+04 3.12771608E+01-1.21236097E+00 6.32471589E-02-1.21281973E-
 05 3
 -2.62654724E-08 1.41075399E-11 1.84352403E+04 3.12771608E+01
 4
 C7H11r_R5_32 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 1.51050085E+00 4.46816837E-02 1.69451550E-05-4.46771106E-08 1.81610987E-
 11 2
 2.01913521E+04 2.23906270E+01 1.51050085E+00 4.46816837E-02 1.69451550E-
 05 3
 -4.46771106E-08 1.81610987E-11 2.01913521E+04 2.23906270E+01
 4
 Ccy(CCJC*CCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.19675207E+00 5.72620518E-02 1.22085954E-05-5.67884663E-08 2.69645910E-
 11 2
 9.56197076E+03 3.65502095E+01-2.19675207E+00 5.72620518E-02 1.22085954E-
 05 3
 -5.67884663E-08 2.69645910E-11 9.56197076E+03 3.65502095E+01
 4
 C7H11r_R5_35 C 7 H 11 G 3E+02 2E+03 1E+03
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 -9.61774964E-01 5.65032897E-02-7.86886612E-06-2.10198712E-08 9.85422456E-
 12 2
 2.04109588E+04 3.35742297E+01-9.61774964E-01 5.65032897E-02-7.86886612E-
 06 3
 -2.10198712E-08 9.85422456E-12 2.04109588E+04 3.35742297E+01
 4
 Ccy(CCJCC*CC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -3.52889657E+00 7.61564940E-02-4.27818663E-05 5.56766936E-09 2.27256826E-
 12 2
 1.82965104E+04 4.13464389E+01-3.52889657E+00 7.61564940E-02-4.27818663E-
 05 3
 5.56766936E-09 2.27256826E-12 1.82965104E+04 4.13464389E+01
 4
 C7H9r_R5_9 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -4.34561862E+00 8.23941626E-02-7.91356628E-05 5.21369945E-08-1.64324915E-
 11 2
 2.29675021E+04 4.49411481E+01-4.34561862E+00 8.23941626E-02-7.91356628E-
 05 3
 5.21369945E-08-1.64324915E-11 2.29675021E+04 4.49411481E+01
 4
 Ccy(CJCC*CC*C) C 7 H 9 G 3E+02 2E+03 1E+03
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 -2.03682909E+00 5.68613706E-02-2.43608298E-06-3.88743420E-08 2.02320509E-
 11 2
 1.70163888E+04 3.57960251E+01-2.03682909E+00 5.68613706E-02-2.43608298E-
 06 3
 -3.88743420E-08 2.02320509E-11 1.70163888E+04 3.57960251E+01
 4
 C7H11r_R5_50 C 7 H 11 G 3E+02 2E+03 1E+03
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-2.55839985E+00 6.28575522E-02-2.15522326E-05-6.36548651E-09 4.18445287E-
 12 2
 1.10773100E+04 3.79749355E+01-2.55839985E+00 6.28575522E-02-2.15522326E-
 05 3
 -6.36548651E-09 4.18445287E-12 1.10773100E+04 3.79749355E+01
 4
 C7H9r_Olef_3 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 8.33188107E-01 5.88829700E-02-1.96850411E-05-2.12398273E-08 1.48731312E-
 11 2
 3.24796389E+04 1.93870636E+01 8.33188107E-01 5.88829700E-02-1.96850411E-
 05 3
 -2.12398273E-08 1.48731312E-11 3.24796389E+04 1.93870636E+01
 4
 C7H11r_Olef_27 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 6.80690007E+00 3.04563718E-02 3.92019900E-05-6.83342930E-08 2.83407164E-
 11 2
 2.83030340E+04 1.09130588E+00 6.80690007E+00 3.04563718E-02 3.92019900E-
 05 3
 -6.83342930E-08 2.83407164E-11 2.83030340E+04 1.09130588E+00
 4
 C7H11r_Olef_2 C 7 H 11 G 3E+02 2E+03 1E+03
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 11 2
 1.93723967E+04 1.72947541E+01 2.21687621E+00 5.74353161E-02-1.47081925E-
 05 3
 -2.06591764E-08 1.26498221E-11 1.93723967E+04 1.72947541E+01
 4
 C7H11r_R5_64 C 7 H 11 G 3E+02 2E+03 1E+03
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 12 2
 1.15411932E+04 3.98265875E+01-3.33120462E+00 7.42597171E-02-4.53781730E-
 05 3
 1.30477263E-08-1.53424306E-12 1.15411932E+04 3.98265875E+01
 4
 C7H11r_R5_23 C 7 H 11 G 3E+02 2E+03 1E+03
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 13 2
 1.05844758E+04 2.88801458E+01-1.39729402E+00 6.63537721E-02-3.48948495E-
 05 3
 7.51761773E-09-6.63376408E-13 1.05844758E+04 2.88801458E+01
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 C7H9r_R5_25 C 7 H 9 G 3E+02 2E+03 1E+03
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 3.44166409E+04 4.65989214E+01-4.65587041E+00 8.45136377E-02-8.31538627E-
 05 3
 5.08867805E-08-1.44116924E-11 3.44166409E+04 4.65989214E+01
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 CJcy(C*CC*CCC) C 7 H 9 G 3E+02 2E+03 1E+03
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 11 2

2.01046519E+04 4.37529792E+01-4.00844099E+00 6.76598728E-02-2.33096057E-
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 C7H10_R5_6 C 7 H 10 G 3E+02 2E+03 1E+03
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 12 2
 8.76057057E+03 3.77188058E+01-2.32818908E+00 6.56962410E-02-4.03115324E-
 05 3
 1.50127480E-08-3.61417492E-12 8.76057057E+03 3.77188058E+01
 4
 C7H11r_R5_20 C 7 H 11 G 3E+02 2E+03 1E+03
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 -2.60768332E+00 7.42550920E-02-4.98253042E-05 1.86408192E-08-3.64565538E-
 12 2
 2.04836462E+04 3.71869126E+01-2.60768332E+00 7.42550920E-02-4.98253042E-
 05 3
 1.86408192E-08-3.64565538E-12 2.04836462E+04 3.71869126E+01
 4
 CJcy(CC*CCCC) C 7 H 11 G 3E+02 2E+03 1E+03
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 12 2
 1.95975116E+04 3.29216454E+01-2.06390101E+00 7.32839142E-02-3.50595367E-
 05 3
 -4.84168416E-09 6.81829590E-12 1.95975116E+04 3.29216454E+01
 4
 C*cy(CCCJCCC) C 7 H 11 G 3E+02 2E+03 1E+03
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 12 2
 1.80245401E+04 3.47711651E+01-1.89295160E+00 6.60337050E-02-2.72672670E-
 05 3
 3.18749675E-09-1.27540535E-12 1.80245401E+04 3.47711651E+01
 4
 C7H10_R5_9 C 7 H 10 G 3E+02 2E+03 1E+03
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 12 2
 9.17572827E+03 4.22190805E+01-3.80725341E+00 7.84785016E-02-6.48049652E-
 05 3
 3.40098636E-08-8.99648405E-12 9.17572827E+03 4.22190805E+01
 4
 C7H9r_Olef_4 C 7 H 9 G 3E+02 2E+03 1E+03
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 11 2
 1.73704210E+04-1.61288093E+00 1.35705467E+00 6.31644674E-02-2.04853080E-
 05 3
 -2.21320627E-08 1.48369285E-11 1.73704210E+04-1.61288093E+00
 4
 C7H11r_R5_38 C 7 H 11 G 3E+02 2E+03 1E+03
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 11 2
 1.95721550E+04 3.01548563E+01 3.93694659E-01 4.25014580E-02 2.59697652E-
 05 3

-5.41032238E-08 2.14700113E-11 1.95721550E+04 3.01548563E+01
 4
 C7H11r_R5_2 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 1.45186924E+00 3.21132014E-02 6.03597513E-05-9.78148336E-08 4.04942782E-
 11 2
 1.19472787E+04 2.55449107E+01 1.45186924E+00 3.21132014E-02 6.03597513E-
 05 3
 -9.78148336E-08 4.04942782E-11 1.19472787E+04 2.55449107E+01
 4
 C7H9r_R5_22 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.39174216E+00 5.85945195E-02 1.72541264E-05-7.67057636E-08 3.84205492E-
 11 2
 1.75664709E+04 3.16956192E+01-2.39174216E+00 5.85945195E-02 1.72541264E-
 05 3
 -7.67057636E-08 3.84205492E-11 1.75664709E+04 3.16956192E+01
 4
 C7H11r_R5_59 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.82718482E+00 6.47547251E-02-9.79397352E-06-3.56965289E-08 2.03992566E-
 11 2
 2.03852523E+04 4.26685050E+01-2.82718482E+00 6.47547251E-02-9.79397352E-
 06 3
 -3.56965289E-08 2.03992566E-11 2.03852523E+04 4.26685050E+01
 4
 C7H11r_Olef C 7 H 11 G 3E+02 2E+03 1E+03
 1
 5.78176040E+00 2.96262891E-02 4.09161992E-05-6.68629688E-08 2.67914387E-
 11 2
 1.74547990E+04 4.60023277E+00 5.78176040E+00 2.96262891E-02 4.09161992E-
 05 3
 -6.68629688E-08 2.67914387E-11 1.74547990E+04 4.60023277E+00
 4
 C7H9r_Olef_1 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 5.02042945E+00 4.69769956E-02-7.12670443E-06-2.34283282E-08 1.28967534E-
 11 2
 3.21095828E+04-1.38081620E+01 5.02042945E+00 4.69769956E-02-7.12670443E-
 06 3
 -2.34283282E-08 1.28967534E-11 3.21095828E+04-1.38081620E+01
 4
 C7H9r_Olef_5 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -5.87673907E-01 6.30721367E-02-2.37119152E-05-1.96073974E-08 1.47193945E-
 11 2
 2.47152399E+04 2.52643921E+01-5.87673907E-01 6.30721367E-02-2.37119152E-
 05 3
 -1.96073974E-08 1.47193945E-11 2.47152399E+04 2.52643921E+01
 4
 C7H11r_R5_41 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 3.41694248E+00 2.78026214E-02 7.40076631E-05-1.17705192E-07 4.94804942E-
 11 2
 2.15585250E+04 1.68783814E+01 3.41694248E+00 2.78026214E-02 7.40076631E-
 05 3
 -1.17705192E-07 4.94804942E-11 2.15585250E+04 1.68783814E+01
 4

C7H11r_Olef_29 C 7 H 11 G 3E+02 2E+03 1E+03
1
1.42716767E+00 5.46939221E-02 1.02256750E-05-5.74888653E-08 2.85183725E-
11 2
2.71758641E+04 2.43428509E+01 1.42716767E+00 5.46939221E-02 1.02256750E-
05 3
-5.74888653E-08 2.85183725E-11 2.71758641E+04 2.43428509E+01
4
C7H11r_Olef_14 C 7 H 11 G 3E+02 2E+03 1E+03
1
2.67287273E+00 5.57934708E-02-1.25346425E-05-2.18501360E-08 1.28591049E-
11 2
1.99660128E+04 1.49878990E+01 2.67287273E+00 5.57934708E-02-1.25346425E-
05 3
-2.18501360E-08 1.28591049E-11 1.99660128E+04 1.49878990E+01
4
C7H11r_R5_54 C 7 H 11 G 3E+02 2E+03 1E+03
1
-6.24489247E-01 5.49516071E-02-1.10689091E-05-1.18955951E-08 5.05531952E-
12 2
1.01205925E+04 2.92257183E+01-6.24489247E-01 5.49516071E-02-1.10689091E-
05 3
-1.18955951E-08 5.05531952E-12 1.01205925E+04 2.92257183E+01
4
CJcy (C*CCCC) C 7 H 11 G 3E+02 2E+03 1E+03
1
-3.18759022E+00 6.28797323E-02 7.44428625E-07-4.66349201E-08 2.36583541E-
11 2
1.10139337E+04 4.06752839E+01-3.18759022E+00 6.28797323E-02 7.44428625E-
07 3
-4.66349201E-08 2.36583541E-11 1.10139337E+04 4.06752839E+01
4
C7H9r_R5_17 C 7 H 9 G 3E+02 2E+03 1E+03
1
-7.29177420E-01 5.82954231E-02-2.52696205E-05-2.05591240E-09 3.18009125E-
12 2
2.84636078E+04 2.87587588E+01-7.29177420E-01 5.82954231E-02-2.52696205E-
05 3
-2.05591240E-09 3.18009125E-12 2.84636078E+04 2.87587588E+01
4
Ccy (C*CC*(C)C) C 7 H 10 G 3E+02 2E+03 1E+03
1
5.83887467E-01 5.01476564E-02 2.75247063E-05-8.02823631E-08 3.82441385E-
11 2
6.35128903E+03 2.04881991E+01 5.83887467E-01 5.01476564E-02 2.75247063E-
05 3
-8.02823631E-08 3.82441385E-11 6.35128903E+03 2.04881991E+01
4
C7H11r_Olef_13 C 7 H 11 G 3E+02 2E+03 1E+03
1
8.60687255E-01 6.91006895E-02-4.59733002E-05 1.11324328E-08 1.35586916E-
12 2
2.67895524E+04 2.61778701E+01 8.60687255E-01 6.91006895E-02-4.59733002E-
05 3
1.11324328E-08 1.35586916E-12 2.67895524E+04 2.61778701E+01
4
Ccy (C*CC (C) *CC) C 7 H 10 G 3E+02 2E+03 1E+03
1

2.03483659E+00 4.78565022E-02 1.01498616E-05-4.87853115E-08 2.38999518E-
 11 2
 6.28693036E+03 1.57940232E+01 2.03483659E+00 4.78565022E-02 1.01498616E-
 05 3
 -4.87853115E-08 2.38999518E-11 6.28693036E+03 1.57940232E+01
 4
 CJcy(CCC*CCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -3.25046613E+00 7.95163768E-02-5.02086670E-05 1.11100255E-08 8.48298321E-
 13 2
 1.98996376E+04 3.87132341E+01-3.25046613E+00 7.95163768E-02-5.02086670E-
 05 3
 1.11100255E-08 8.48298321E-13 1.98996376E+04 3.87132341E+01
 4
 C7H11r_R5_48 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -3.33120462E+00 7.42597171E-02-4.53781730E-05 1.30477263E-08-1.53424306E-
 12 2
 1.15411932E+04 3.87279752E+01-3.33120462E+00 7.42597171E-02-4.53781730E-
 05 3
 1.30477263E-08-1.53424306E-12 1.15411932E+04 3.87279752E+01
 4
 C7H11r_R5_12 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.42111821E+00 6.80226294E-02-3.46761739E-05 2.68910952E-09 2.32434220E-
 12 2
 2.01815202E+04 3.13953239E+01-1.42111821E+00 6.80226294E-02-3.46761739E-
 05 3
 2.68910952E-09 2.32434220E-12 2.01815202E+04 3.13953239E+01
 4
 C7H10_R5_5 C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -2.79695434E+00 6.57228126E-02-2.04924193E-05-2.28784645E-08 1.55433727E-
 11 2
 1.16367980E+04 3.97632240E+01-2.79695434E+00 6.57228126E-02-2.04924193E-
 05 3
 -2.28784645E-08 1.55433727E-11 1.16367980E+04 3.97632240E+01
 4
 C7H11r_Olef_10 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -8.20115501E-01 7.59751859E-02-5.71916864E-05 2.04275178E-08-1.66677324E-
 12 2
 1.87684625E+04 3.06974086E+01-8.20115501E-01 7.59751859E-02-5.71916864E-
 05 3
 2.04275178E-08-1.66677324E-12 1.87684625E+04 3.06974086E+01
 4
 C7H9r_R5_2 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -9.40793031E-01 5.63033653E-02-1.20718321E-07-4.52087120E-08 2.40763624E-
 11 2
 1.75021122E+04 2.81000556E+01-9.40793031E-01 5.63033653E-02-1.20718321E-
 07 3
 -4.52087120E-08 2.40763624E-11 1.75021122E+04 2.81000556E+01
 4
 C7H9r_R5_1 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -5.18382157E+00 7.50013814E-02-1.45443248E-05-4.99151840E-08 2.99976285E-
 11 2

1.90201853E+04 4.43302479E+01-5.18382157E+00 7.50013814E-02-1.45443248E-
 05 3
 -4.99151840E-08 2.99976285E-11 1.90201853E+04 4.43302479E+01
 4
 C*cy(CCC*CCJC) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -3.78509370E+00 7.75751992E-02-5.77171876E-05 2.19640280E-08-3.55023512E-
 12 2
 2.59290351E+04 3.93755127E+01-3.78509370E+00 7.75751992E-02-5.77171876E-
 05 3
 2.19640280E-08-3.55023512E-12 2.59290351E+04 3.93755127E+01
 4
 C7H9r_R5_5 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.32818908E+00 6.56962410E-02-4.03115324E-05 1.50127480E-08-3.61417492E-
 12 2
 2.32894550E+04 3.77188058E+01-2.32818908E+00 6.56962410E-02-4.03115324E-
 05 3
 1.50127480E-08-3.61417492E-12 2.32894550E+04 3.77188058E+01
 4
 C7H11r_R5_7 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.47620812E+00 6.16127017E-02-1.89835425E-05-1.05435298E-08 6.24157762E-
 12 2
 1.26108124E+04 3.34955099E+01-1.47620812E+00 6.16127017E-02-1.89835425E-
 05 3
 -1.05435298E-08 6.24157762E-12 1.26108124E+04 3.34955099E+01
 4
 C7H10_R5_11 C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -1.72037100E+00 6.42273900E-02-3.17474329E-05 2.53158604E-09 1.74607596E-
 12 2
 1.26203222E+04 3.45217671E+01-1.72037100E+00 6.42273900E-02-3.17474329E-
 05 3
 2.53158604E-09 1.74607596E-12 1.26203222E+04 3.45217671E+01
 4
 C7H11r_R5_63 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -8.82752989E-01 6.41069685E-02-2.03454762E-05-1.54380214E-08 9.76034967E-
 12 2
 2.09186309E+04 2.79801091E+01-8.82752989E-01 6.41069685E-02-2.03454762E-
 05 3
 -1.54380214E-08 9.76034967E-12 2.09186309E+04 2.79801091E+01
 4
 C7H10_R5_13 C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -1.24096459E-01 5.97777101E-02-3.02319742E-05 5.89041996E-09-4.57668048E-
 13 2
 9.71334531E+03 2.54121198E+01-1.24096459E-01 5.97777101E-02-3.02319742E-
 05 3
 5.89041996E-09-4.57668048E-13 9.71334531E+03 2.54121198E+01
 4
 CJCcyC*CC*CC C 7 H 9 G 3E+02 2E+03 1E+03
 1
 2.09540430E+00 4.00261919E-02 4.53995620E-05-9.75886060E-08 4.45451927E-
 11 2
 3.31166197E+04 1.67551221E+01 2.09540430E+00 4.00261919E-02 4.53995620E-
 05 3

-9.75886060E-08 4.45451927E-11 3.31166197E+04 1.67551221E+01
 4
 Ccy(C*CCC*C(C)) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 3.48578572E+00 4.55653480E-02-7.22498316E-06-1.72882599E-08 9.55576502E-
 12 2
 6.22257170E+03 9.71355295E+00 3.48578572E+00 4.55653480E-02-7.22498316E-
 06 3
 -1.72882599E-08 9.55576502E-12 6.22257170E+03 9.71355295E+00
 4
 Ccy(C*CCCCJC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.59498597E+00 6.82505489E-02-3.22985428E-05 3.75607913E-11 3.14343490E-
 12 2
 1.73397930E+04 3.21917567E+01-1.59498597E+00 6.82505489E-02-3.22985428E-
 05 3
 3.75607913E-11 3.14343490E-12 1.73397930E+04 3.21917567E+01
 4
 CC*cy(CCJCC*C) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -2.61461669E+00 6.61468588E-02-4.45484079E-05 1.85910422E-08-4.58109438E-
 12 2
 2.51415495E+04 3.75545482E+01-2.61461669E+00 6.61468588E-02-4.45484079E-
 05 3
 1.85910422E-08-4.58109438E-12 2.51415495E+04 3.75545482E+01
 4
 Ccy(C*CCJCC*C) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -1.83765502E+00 5.63389193E-02-2.45134730E-06-3.79963867E-08 1.96926355E-
 11 2
 1.76833966E+04 3.72264500E+01-1.83765502E+00 5.63389193E-02-2.45134730E-
 06 3
 -3.79963867E-08 1.96926355E-11 1.76833966E+04 3.72264500E+01
 4
 Ccy(C*CCCJCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.59498597E+00 6.82505489E-02-3.22985428E-05 3.75607913E-11 3.14343490E-
 12 2
 1.73397930E+04 3.21917567E+01-1.59498597E+00 6.82505489E-02-3.22985428E-
 05 3
 3.75607913E-11 3.14343490E-12 1.73397930E+04 3.21917567E+01
 4
 C7H11r_Olef_17 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 1.94187680E+00 5.76703114E-02-3.99151624E-06-3.94925432E-08 2.12540709E-
 11 2
 2.51435057E+04 1.82659216E+01 1.94187680E+00 5.76703114E-02-3.99151624E-
 06 3
 -3.94925432E-08 2.12540709E-11 2.51435057E+04 1.82659216E+01
 4
 C*cy(CCC*CCC) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -3.49866609E+00 7.71245815E-02-5.34803120E-05 1.83857337E-08-2.58331567E-
 12 2
 9.54805617E+03 3.91343052E+01-3.49866609E+00 7.71245815E-02-5.34803120E-
 05 3
 1.83857337E-08-2.58331567E-12 9.54805617E+03 3.91343052E+01
 4

C7H11r_R5_33 C 7 H 11 G 3E+02 2E+03 1E+03
1
5.03220597E-01 5.36307099E-02-1.46536536E-07-3.14292247E-08 1.43999522E-
11 2
2.17119600E+04 2.58425833E+01 5.03220597E-01 5.36307099E-02-1.46536536E-
07 3
-3.14292247E-08 1.43999522E-11 2.17119600E+04 2.58425833E+01
4
C7H11r_R5_47 C 7 H 11 G 3E+02 2E+03 1E+03
1
-1.47171520E+00 5.07528934E-02 2.40446578E-05-6.87798815E-08 3.20150434E-
11 2
1.95464484E+04 3.92491315E+01-1.47171520E+00 5.07528934E-02 2.40446578E-
05 3
-6.87798815E-08 3.20150434E-11 1.95464484E+04 3.92491315E+01
4
C7H11r_Olef_18 C 7 H 11 G 3E+02 2E+03 1E+03
1
4.78947053E+00 4.71542934E-02 3.77859532E-07-3.12100465E-08 1.55223998E-
11 2
2.79810811E+04 8.31364814E+00 4.78947053E+00 4.71542934E-02 3.77859532E-
07 3
-3.12100465E-08 1.55223998E-11 2.79810811E+04 8.31364814E+00
4
C7H9r_R5_8 C 7 H 9 G 3E+02 2E+03 1E+03
1
3.19935811E+00 4.60159658E-02-1.14618587E-05-1.37099657E-08 8.58884557E-
12 2
2.26035506E+04 9.54929534E+00 3.19935811E+00 4.60159658E-02-1.14618587E-
05 3
-1.37099657E-08 8.58884557E-12 2.26035506E+04 9.54929534E+00
4
C7H10_R5_10 C 7 H 10 G 3E+02 2E+03 1E+03
1
1.89333308E+00 4.30797885E-02 8.59215625E-06-3.12338266E-08 1.23606486E-
11 2
1.00352983E+04 1.81897776E+01 1.89333308E+00 4.30797885E-02 8.59215625E-
06 3
-3.12338266E-08 1.23606486E-11 1.00352983E+04 1.81897776E+01
4
Ccy(CC(C)*CC*C) C 7 H 10 G 3E+02 2E+03 1E+03
1
-2.20819195E+00 6.65545183E-02-4.27374495E-06-5.34917836E-08 2.98212179E-
11 2
7.80500348E+03 3.31228279E+01-2.20819195E+00 6.65545183E-02-4.27374495E-
06 3
-5.34917836E-08 2.98212179E-11 7.80500348E+03 3.31228279E+01
4
C7H9r_R5_12 C 7 H 9 G 3E+02 2E+03 1E+03
1
-1.32574494E+00 7.08041780E-02-6.00668768E-05 3.34359042E-08-9.48448857E-
12 2
3.59060538E+04 3.01037725E+01-1.32574494E+00 7.08041780E-02-6.00668768E-
05 3
3.34359042E-08-9.48448857E-12 3.59060538E+04 3.01037725E+01
4
C7H11r_R5_46 C 7 H 11 G 3E+02 2E+03 1E+03
1

-8.61240304E-02 5.10359462E-02 3.26178858E-06-3.00227260E-08 1.24913270E-11 2
1.08577032E+04 2.54050384E+01-8.61240304E-02 5.10359462E-02 3.26178858E-06 3
-3.00227260E-08 1.24913270E-11 1.08577032E+04 2.54050384E+01
4
C7H10_R6 C 7 H 10 G 3E+02 2E+03 1E+03
1
-3.11638473E+00 5.89138828E-02 2.88856077E-06-4.67277655E-08 2.33780523E-11 2
6.39982008E+03 3.98731147E+01-3.11638473E+00 5.89138828E-02 2.88856077E-06 3
-4.67277655E-08 2.33780523E-11 6.39982008E+03 3.98731147E+01
4
C7H9r_R5_21 C 7 H 9 G 3E+02 2E+03 1E+03
1
-1.06723230E+00 5.63111349E-02-1.97401458E-05-7.43438688E-09 4.97496870E-12 2
3.63589695E+04 3.41719302E+01-1.06723230E+00 5.63111349E-02-1.97401458E-05 3
-7.43438688E-09 4.97496870E-12 3.63589695E+04 3.41719302E+01
4
Ccy (CC*CCC*C) C 7 H 10 G 3E+02 2E+03 1E+03
1
3.42999852E+00 5.23573898E-02-9.09025304E-06-2.41832329E-08 1.35006533E-11 2
7.37058875E+03-5.86518587E+00 3.42999852E+00 5.23573898E-02-9.09025304E-06 3
-2.41832329E-08 1.35006533E-11 7.37058875E+03-5.86518587E+00
4
C7H9r_R5_18 C 7 H 9 G 3E+02 2E+03 1E+03
1
-1.40814080E+00 5.64410714E-02-1.27201345E-05-1.87817227E-08 1.00184833E-11 2
2.87034168E+04 3.33939016E+01-1.40814080E+00 5.64410714E-02-1.27201345E-05 3
-1.87817227E-08 1.00184833E-11 2.87034168E+04 3.33939016E+01
4
C7H11r_R5_6 C 7 H 11 G 3E+02 2E+03 1E+03
1
-8.61240304E-02 5.10359462E-02 3.26178858E-06-3.00227260E-08 1.24913270E-11 2
1.08577032E+04 2.60981856E+01-8.61240304E-02 5.10359462E-02 3.26178858E-06 3
-3.00227260E-08 1.24913270E-11 1.08577032E+04 2.60981856E+01
4
C7H10_R5_2 C 7 H 10 G 3E+02 2E+03 1E+03
1
-2.42127982E+00 6.80022431E-02-4.46060255E-05 1.80186603E-08-4.35688152E-12 2
9.96905739E+03 3.82897952E+01-2.42127982E+00 6.80022431E-02-4.46060255E-05 3
1.80186603E-08-4.35688152E-12 9.96905739E+03 3.82897952E+01
4
C7H9r_R5_7 C 7 H 9 G 3E+02 2E+03 1E+03
1
-2.70770743E+00 6.84528609E-02-4.88429010E-05 2.15969545E-08-5.32380097E-12 2

2.63500363E+04 3.85310027E+01-2.70770743E+00 6.84528609E-02-4.88429010E-
 05 3
 2.15969545E-08-5.32380097E-12 2.63500363E+04 3.85310027E+01
 4
 C7H9r_Olef_2 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -3.37975333E+00 7.94789987E-02-5.55103665E-05 7.18318219E-09 6.29647382E-
 12 2
 2.61689543E+04 3.72058737E+01-3.37975333E+00 7.94789987E-02-5.55103665E-
 05 3
 7.18318219E-09 6.29647382E-12 2.61689543E+04 3.72058737E+01
 4
 CCcyCJC*CC*C C 7 H 9 G 3E+02 2E+03 1E+03
 1
 1.27814058E+00 5.84233970E-02-4.57400094E-06-4.01932102E-08 2.17418825E-
 11 2
 1.93967576E+04 2.19155300E+00 1.27814058E+00 5.84233970E-02-4.57400094E-
 06 3
 -4.01932102E-08 2.17418825E-11 1.93967576E+04 2.19155300E+00
 4
 C7H11r_R5_56 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 4.00650423E-01 5.57816898E-02-1.27831183E-05-1.33669193E-08 6.60459720E-
 12 2
 2.09688276E+04 2.64099386E+01 4.00650423E-01 5.57816898E-02-1.27831183E-
 05 3
 -1.33669193E-08 6.60459720E-12 2.09688276E+04 2.64099386E+01
 4
 C7H10_R5_1 C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -2.83574055E+00 7.39625243E-02-6.39059776E-05 3.48390542E-08-8.15603623E-
 12 2
 9.87899215E+03 4.06104530E+01-2.83574055E+00 7.39625243E-02-6.39059776E-
 05 3
 3.48390542E-08-8.15603623E-12 9.87899215E+03 4.06104530E+01
 4
 C7H9r_R5_10 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -4.10524067E-01 6.02283279E-02-3.44688497E-05 9.46871421E-09-1.42458750E-
 12 2
 2.60943242E+04 2.63464745E+01-4.10524067E-01 6.02283279E-02-3.44688497E-
 05 3
 9.46871421E-09-1.42458750E-12 2.60943242E+04 2.63464745E+01
 4
 C7H11r_R5_37 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -5.36641810E-01 5.32458288E-02-2.73937990E-06-2.40877970E-08 1.04373898E-
 11 2
 1.99684809E+04 3.22113183E+01-5.36641810E-01 5.32458288E-02-2.73937990E-
 06 3
 -2.40877970E-08 1.04373898E-11 1.99684809E+04 3.22113183E+01
 4
 Ccy(CJCC*CCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.17342695E+00 6.21546622E-02-8.94323499E-06-2.75156833E-08 1.38883550E-
 11 2
 1.74577066E+04 3.79270655E+01-2.17342695E+00 6.21546622E-02-8.94323499E-
 06 3

-2.75156833E-08 1.38883550E-11 1.74577066E+04 3.79270655E+01
 4
 Ccy(CJC*CCCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -9.70910672E-01 5.00369810E-02 2.68489125E-05-6.97579787E-08 3.12728516E-
 11 2
 8.34505322E+03 3.17893281E+01-9.70910672E-01 5.00369810E-02 2.68489125E-
 05 3
 -6.97579787E-08 3.12728516E-11 8.34505322E+03 3.17893281E+01
 4
 Ccy(CCC*CCJC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.37126841E+00 5.90549486E-02 7.09018752E-06-5.09783178E-08 2.46745033E-
 11 2
 9.34269182E+03 3.71806279E+01-2.37126841E+00 5.90549486E-02 7.09018752E-
 06 3
 -5.09783178E-08 2.46745033E-11 9.34269182E+03 3.71806279E+01
 4
 C7H11r_R5_57 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -1.53064414E+00 5.68933775E-02-8.55987216E-06-1.99848896E-08 9.39440131E-
 12 2
 1.80417152E+04 3.64007441E+01-1.53064414E+00 5.68933775E-02-8.55987216E-
 06 3
 -1.99848896E-08 9.39440131E-12 1.80417152E+04 3.64007441E+01
 4
 C*CCCCJC*C C 7 H 11 G 3E+02 2E+03 1E+03
 1
 1.86542471E+00 5.34871379E-02-8.69980189E-07-3.59423628E-08 1.83151136E-
 11 2
 2.19151721E+04 2.27296346E+01 1.86542471E+00 5.34871379E-02-8.69980189E-
 07 3
 -3.59423628E-08 1.83151136E-11 2.19151721E+04 2.27296346E+01
 4
 C*Ccy(C*CCCJC) C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -1.76814112E+00 6.00859880E-02-3.25987385E-05 8.05268737E-09-1.12798879E-
 12 2
 3.37077048E+04 3.79399583E+01-1.76814112E+00 6.00859880E-02-3.25987385E-
 05 3
 8.05268737E-09-1.12798879E-12 3.37077048E+04 3.79399583E+01
 4
 C7H11r_Olef_7 C 7 H 11 G 3E+02 2E+03 1E+03
 1
 1.27622813E+00 6.40183346E-02-3.42788630E-05 1.36441879E-09 4.24658933E-
 12 2
 1.70640788E+04 1.95528494E+01 1.27622813E+00 6.40183346E-02-3.42788630E-
 05 3
 1.36441879E-09 4.24658933E-12 1.70640788E+04 1.95528494E+01
 4
 C*cy(CCCCJCC) C 7 H 11 G 3E+02 2E+03 1E+03
 1
 -2.04869181E+00 6.49459760E-02-2.14276190E-05-4.98840562E-09 2.25269220E-
 12 2
 1.83828768E+04 3.58854896E+01-2.04869181E+00 6.49459760E-02-2.14276190E-
 05 3
 -4.98840562E-09 2.25269220E-12 1.83828768E+04 3.58854896E+01
 4

C7H11r_R5_36 C 7 H 11 G 3E+02 2E+03 1E+03
1
-1.96905522E+00 6.54523159E-02-2.49605577E-05-7.77198528E-09 6.09307809E-
12 2
2.19315667E+04 3.70261860E+01-1.96905522E+00 6.54523159E-02-2.49605577E-
05 3
-7.77198528E-09 6.09307809E-12 2.19315667E+04 3.70261860E+01
4
CJCcyC*CCC*C C 7 H 9 G 3E+02 2E+03 1E+03
1
3.54635343E+00 3.77350377E-02 2.80247173E-05-6.60915544E-08 3.02010059E-
11 2
3.30522611E+04 1.13677990E+01 3.54635343E+00 3.77350377E-02 2.80247173E-
05 3
-6.60915544E-08 3.02010059E-11 3.30522611E+04 1.13677990E+01
4
C7H11r_R5_19 C 7 H 11 G 3E+02 2E+03 1E+03
1
3.41694248E+00 2.78026214E-02 7.40076631E-05-1.17705192E-07 4.94804942E-
11 2
2.15585250E+04 1.68783814E+01 3.41694248E+00 2.78026214E-02 7.40076631E-
05 3
-1.17705192E-07 4.94804942E-11 2.15585250E+04 1.68783814E+01
4
CJCcyCC*CC*C C 7 H 9 G 3E+02 2E+03 1E+03
1
-1.13247016E+00 5.81977349E-02 1.19069949E-05-7.07332009E-08 3.64816196E-
11 2
3.45763559E+04 3.01581688E+01-1.13247016E+00 5.81977349E-02 1.19069949E-
05 3
-7.07332009E-08 3.64816196E-11 3.45763559E+04 3.01581688E+01
4
C7H11r_R5_16 C 7 H 11 G 3E+02 2E+03 1E+03
1
-3.54909004E-01 5.29331191E-02 1.50200476E-05-5.93537683E-08 2.87061307E-
11 2
2.01656455E+04 3.07917551E+01-3.54909004E-01 5.29331191E-02 1.50200476E-
05 3
-5.93537683E-08 2.87061307E-11 2.01656455E+04 3.07917551E+01
4
CJcy(C*CCC*CC) C 7 H 9 G 3E+02 2E+03 1E+03
1
5.93565033E+00 3.64011456E-02 1.84713227E-05-4.73955182E-08 2.09566545E-
11 2
2.22978532E+04-1.68723127E+01 5.93565033E+00 3.64011456E-02 1.84713227E-
05 3
-4.73955182E-08 2.09566545E-11 2.22978532E+04-1.68723127E+01
4
C7H11r_Olef_12 C 7 H 11 G 3E+02 2E+03 1E+03
1
3.39282593E+00 5.53791572E-02-2.13663610E-05-7.99549166E-09 6.90988419E-
12 2
2.50791470E+04 1.28785985E+01 3.39282593E+00 5.53791572E-02-2.13663610E-
05 3
-7.99549166E-09 6.90988419E-12 2.50791470E+04 1.28785985E+01
4
C7H9r_Olef_12 C 7 H 9 G 3E+02 2E+03 1E+03
1

2.80800380E+00 6.08733132E-02-3.78601527E-05 9.36498890E-09 4.92741773E-
13 2
1.73060623E+04-6.30705684E+00 2.80800380E+00 6.08733132E-02-3.78601527E-
05 3
9.36498890E-09 4.92741773E-13 1.73060623E+04-6.30705684E+00
4
C7H11r_Olef_20 C 7 H 11 G 3E+02 2E+03 1E+03
1
3.39282593E+00 5.53791572E-02-2.13663610E-05-7.99549166E-09 6.90988419E-
12 2
2.50791470E+04 1.28785985E+01 3.39282593E+00 5.53791572E-02-2.13663610E-
05 3
-7.99549166E-09 6.90988419E-12 2.50791470E+04 1.28785985E+01
4
C7H11r_R5_13 C 7 H 11 G 3E+02 2E+03 1E+03
1
1.12415532E+00 4.01508585E-02 3.95134804E-05-7.83508840E-08 3.40884398E-
11 2
1.97504878E+04 2.55983333E+01 1.12415532E+00 4.01508585E-02 3.95134804E-
05 3
-7.83508840E-08 3.40884398E-11 1.97504878E+04 2.55983333E+01
4
C*cy(CC*CCCJC) C 7 H 9 G 3E+02 2E+03 1E+03
1
-4.33526273E+00 7.97391922E-02-6.75117386E-05 3.46402279E-08-8.70964510E-
12 2
3.15932564E+04 4.50190203E+01-4.33526273E+00 7.97391922E-02-6.75117386E-
05 3
3.46402279E-08-8.70964510E-12 3.15932564E+04 4.50190203E+01
4
C7H11r_R5_5 C 7 H 11 G 3E+02 2E+03 1E+03
1
-1.42111821E+00 6.80226294E-02-3.46761739E-05 2.68910952E-09 2.32434220E-
12 2
2.01815202E+04 3.13953239E+01-1.42111821E+00 6.80226294E-02-3.46761739E-
05 3
2.68910952E-09 2.32434220E-12 2.01815202E+04 3.13953239E+01
4
C7H11r_R5_28 C 7 H 11 G 3E+02 2E+03 1E+03
1
-8.58928807E-01 6.24381111E-02-2.05641519E-05-1.06095131E-08 6.77263106E-
12 2
1.13215865E+04 2.79498376E+01-8.58928807E-01 6.24381111E-02-2.05641519E-
05 3
-1.06095131E-08 6.77263106E-12 1.13215865E+04 2.79498376E+01
4
C7H11r_R5_73 C 7 H 11 G 3E+02 2E+03 1E+03
1
-2.79283941E+00 7.03440562E-02-3.10474753E-05-5.07940456E-09 5.90176441E-
12 2
1.22783039E+04 3.53127604E+01-2.79283941E+00 7.03440562E-02-3.10474753E-
05 3
-5.07940456E-09 5.90176441E-12 1.22783039E+04 3.53127604E+01
4
C7H11r_R5_52 C 7 H 11 G 3E+02 2E+03 1E+03
1
-4.13837951E-01 5.90736032E-02-1.75844824E-05-1.05587764E-08 6.08548867E-
12 2

1.86609123E+04 2.79433676E+01-4.13837951E-01 5.90736032E-02-1.75844824E-
05 3
-1.05587764E-08 6.08548867E-12 1.86609123E+04 2.79433676E+01
4
C7H11r_R5_8 C 7 H 11 G 3E+02 2E+03 1E+03
1
-8.58928807E-01 6.24381111E-02-2.05641519E-05-1.06095131E-08 6.77263106E-
12 2
1.13215865E+04 2.79498376E+01-8.58928807E-01 6.24381111E-02-2.05641519E-
05 3
-1.06095131E-08 6.77263106E-12 1.13215865E+04 2.79498376E+01
4
C7H10_R5_4 C 7 H 10 G 3E+02 2E+03 1E+03
1
-4.34561862E+00 8.23941626E-02-7.91356628E-05 5.21369945E-08-1.64324915E-
11 2
8.43861761E+03 4.49411481E+01-4.34561862E+00 8.23941626E-02-7.91356628E-
05 3
5.21369945E-08-1.64324915E-11 8.43861761E+03 4.49411481E+01
4
C7H11r_R5_44 C 7 H 11 G 3E+02 2E+03 1E+03
1
-1.47620812E+00 6.16127017E-02-1.89835425E-05-1.05435298E-08 6.24157762E-
12 2
1.26108124E+04 3.34955099E+01-1.47620812E+00 6.16127017E-02-1.89835425E-
05 3
-1.05435298E-08 6.24157762E-12 1.26108124E+04 3.34955099E+01
4
Ccy(CC*CC*CC) C 7 H 10 G 3E+02 2E+03 1E+03
1
-2.34112559E+00 5.66007888E-02 5.28941846E-06-4.72416374E-08 2.30893636E-
11 2
7.27300372E+03 3.65071536E+01-2.34112559E+00 5.66007888E-02 5.28941846E-
06 3
-4.72416374E-08 2.30893636E-11 7.27300372E+03 3.65071536E+01
4
C7H10_R5_8 C 7 H 10 G 3E+02 2E+03 1E+03
1
-2.91617588E+00 7.61845721E-02-6.20304254E-05 3.26809995E-08-8.88058869E-
12 2
1.11670598E+04 3.73536014E+01-2.91617588E+00 7.61845721E-02-6.20304254E-
05 3
3.26809995E-08-8.88058869E-12 1.11670598E+04 3.73536014E+01
4
CCC*CC*CCJ C 7 H 11 G 3E+02 2E+03 1E+03
1
-6.06754211E-01 5.47996470E-02 2.25984857E-05-7.37950950E-08 3.48526981E-
11 2
1.19416465E+04 3.05994406E+01-6.06754211E-01 5.47996470E-02 2.25984857E-
05 3
-7.37950950E-08 3.48526981E-11 1.19416465E+04 3.05994406E+01
4
C7H11r_R5_74 C 7 H 11 G 3E+02 2E+03 1E+03
1
1.51050085E+00 4.46816837E-02 1.69451550E-05-4.46771106E-08 1.81610987E-
11 2
2.01913521E+04 2.23906270E+01 1.51050085E+00 4.46816837E-02 1.69451550E-
05 3

-4.46771106E-08 1.81610987E-11 2.01913521E+04 2.23906270E+01
4
C7H11r_R5_25 C 7 H 11 G 3E+02 2E+03 1E+03
1
-9.92278928E-01 5.29777165E-02 5.77082548E-06-3.81120204E-08 1.68304088E-
11 2
1.87788259E+04 3.36786765E+01-9.92278928E-01 5.29777165E-02 5.77082548E-
06 3
-3.81120204E-08 1.68304088E-11 1.87788259E+04 3.36786765E+01
4
C7H9r_Olef_16 C 7 H 9 G 3E+02 2E+03 1E+03
1
-6.17761019E-01 6.11741242E-02-2.31019634E-06-5.27368788E-08 2.92173180E-
11 2
3.25439975E+04 2.47743867E+01-6.17761019E-01 6.11741242E-02-2.31019634E-
06 3
-5.27368788E-08 2.92173180E-11 3.25439975E+04 2.47743867E+01
4
C7H10_R5_15 C 7 H 10 G 3E+02 2E+03 1E+03
1
-3.80725341E+00 7.84785016E-02-6.48049652E-05 3.40098636E-08-8.99648405E-
12 2
9.17572827E+03 4.22190805E+01-3.80725341E+00 7.84785016E-02-6.48049652E-
05 3
3.40098636E-08-8.99648405E-12 9.17572827E+03 4.22190805E+01
4
C7H11r_Olef_23 C 7 H 11 G 3E+02 2E+03 1E+03
1
2.16025388E+00 5.70889001E-02-9.85053374E-06-2.92462444E-08 1.66981534E-
11 2
2.91429329E+04 2.10407690E+01 2.16025388E+00 5.70889001E-02-9.85053374E-
06 3
-2.92462444E-08 1.66981534E-11 2.91429329E+04 2.10407690E+01
4
Ccy(C*CCCCJ) C 7 H 11 G 3E+02 2E+03 1E+03
1
-1.06506294E+00 5.20056187E-02 2.15616747E-05-6.43118253E-08 2.92595343E-
11 2
9.18808453E+03 3.34494813E+01-1.06506294E+00 5.20056187E-02 2.15616747E-
05 3
-6.43118253E-08 2.92595343E-11 9.18808453E+03 3.34494813E+01
4
C7H11r_R5_24 C 7 H 11 G 3E+02 2E+03 1E+03
1
-4.57727715E-01 5.79868992E-02-1.86506870E-05-6.02664942E-09 3.53243577E-
12 2
1.79421443E+04 2.69028070E+01-4.57727715E-01 5.79868992E-02-1.86506870E-
05 3
-6.02664942E-09 3.53243577E-12 1.79421443E+04 2.69028070E+01
4
C7H9r_R5_16 C 7 H 9 G 3E+02 2E+03 1E+03
1
-4.65587041E+00 8.45136377E-02-8.31538627E-05 5.08867805E-08-1.44116924E-
11 2
3.44166409E+04 4.65989214E+01-4.65587041E+00 8.45136377E-02-8.31538627E-
05 3
5.08867805E-08-1.44116924E-11 3.44166409E+04 4.65989214E+01
4

C7H9r_Olef_6 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 2.03483659E+00 4.78565022E-02 1.01498616E-05-4.87853115E-08 2.38999518E-
 11 2
 2.08158148E+04 1.57940232E+01 2.03483659E+00 4.78565022E-02 1.01498616E-
 05 3
 -4.87853115E-08 2.38999518E-11 2.08158148E+04 1.57940232E+01
 4
 C7H9r_R5_4 C 7 H 9 G 3E+02 2E+03 1E+03
 1
 -3.18109710E+00 8.05536262E-02-1.00747383E-04 8.72123403E-08-3.17435977E-
 11 2
 2.47552378E+04 4.04881797E+01-3.18109710E+00 8.05536262E-02-1.00747383E-
 04 3
 8.72123403E-08-3.17435977E-11 2.47552378E+04 4.04881797E+01
 4
 Ccy(C*CC*CCC) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -1.27319430E+00 5.06742272E-02 1.71454250E-05-5.77914023E-08 2.66216076E-
 11 2
 5.95996607E+03 3.20205700E+01-1.27319430E+00 5.06742272E-02 1.71454250E-
 05 3
 -5.77914023E-08 2.66216076E-11 5.95996607E+03 3.20205700E+01
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 C7H11r_R5_43 C 7 H 11 G 3E+02 2E+03 1E+03
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 -5.10649219E-01 5.18453901E-02 2.08596955E-05-6.75296707E-08 3.22342282E-
 11 2
 2.05239821E+04 3.25992268E+01-5.10649219E-01 5.18453901E-02 2.08596955E-
 05 3
 -6.75296707E-08 3.22342282E-11 2.05239821E+04 3.25992268E+01
 4
 CJcy(CC*CC*CC) C 7 H 9 G 3E+02 2E+03 1E+03
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 2.39354856E-01 6.29776096E-02-1.28388456E-05-3.74745035E-08 2.23137364E-
 11 2
 3.26690202E+04 8.76745727E+00 2.39354856E-01 6.29776096E-02-1.28388456E-
 05 3
 -3.74745035E-08 2.23137364E-11 3.26690202E+04 8.76745727E+00
 4
 C7H11r_R5_11 C 7 H 11 G 3E+02 2E+03 1E+03
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 -2.54875437E+00 6.81146079E-02-1.72207743E-05-3.01541727E-08 1.89749867E-
 11 2
 2.19883794E+04 4.00353001E+01-2.54875437E+00 6.81146079E-02-1.72207743E-
 05 3
 -3.01541727E-08 1.89749867E-11 2.19883794E+04 4.00353001E+01
 4
 C7H8 Toluene g 1/93C 7.H 8. 0. 0.G 200.000 6000.000 1000.
 1
 1.29393610E+01 2.66922277E-02-9.68422041E-06 1.57392386E-09-9.46671699E-
 14 2
 -6.76971149E+02-4.67249759E+01 1.61200102E+00 2.11179855E-02 8.53239986E-
 05 3
 -1.32568501E-07 5.59411406E-11 4.09654820E+03 2.02969771E+01
 6.03402967E+03 4
 C6H9O2r_R5_3 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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-6.00112368E+00 1.17521096E-01-1.60427909E-04 1.28519839E-07-4.33140080E-11 2
1.34562497E+04 5.15959016E+01-6.00112368E+00 1.17521096E-01-1.60427909E-04 3
1.28519839E-07-4.33140080E-11 1.34562497E+04 5.15959016E+01 4
C6H7O2r_Olef_1 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
1
2.51898885E+00 7.74164029E-02-9.70215222E-05 7.38778494E-08-2.41187052E-11 2
1.78579805E+04-1.93159366E+00 2.51898885E+00 7.74164029E-02-9.70215222E-05 3
7.38778494E-08-2.41187052E-11 1.78579805E+04-1.93159366E+00 4
C6H12O3_Olef_2 C 6 O 3 H 12 G 3E+02 2E+03 1E+03
1
2.72946179E+00 8.89993281E-02-8.78628279E-05 5.57505584E-08-1.65922733E-11 2
-3.91503378E+04 2.02539608E+01 2.72946179E+00 8.89993281E-02-8.78628279E-05 3
5.57505584E-08-1.65922733E-11-3.91503378E+04 2.02539608E+01 4
C6H7O2r_Olef_3 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
1
-2.24338083E+00 8.08771031E-02-6.88257200E-05 2.44301233E-08-1.49757124E-12 2
2.05239759E+04 3.69701437E+01-2.24338083E+00 8.08771031E-02-6.88257200E-05 3
2.44301233E-08-1.49757124E-12 2.05239759E+04 3.69701437E+01 4
C6H12O2_Olef_2 C 6 O 2 H 12 G 3E+02 2E+03 1E+03
1
1.55061611E+00 8.98405491E-02-8.97493185E-05 5.59368647E-08-1.61612406E-11 2
-1.97138774E+04 2.10034206E+01 1.55061611E+00 8.98405491E-02-8.97493185E-05 3
5.59368647E-08-1.61612406E-11-1.97138774E+04 2.10034206E+01 4
C5H6O2_Olef C 5 O 2 H 6 G 3E+02 2E+03 1E+03
1
-2.79478493E+00 7.65827124E-02-6.02966205E-05 1.15175037E-08 4.36233414E-12 2
4.64833540E+03 3.49088112E+01-2.79478493E+00 7.65827124E-02-6.02966205E-05 3
1.15175037E-08 4.36233414E-12 4.64833540E+03 3.49088112E+01 4
CC(OH)CC*CC*O C 6 O 2 H 10 G 3E+02 2E+03 1E+03
1
-2.19969455E+00 1.05485445E-01-1.32868803E-04 9.83458509E-08-3.03384693E-11 2
-4.18139958E+04 3.77589230E+01-2.19969455E+00 1.05485445E-01-1.32868803E-04 3
9.83458509E-08-3.03384693E-11-4.18139958E+04 3.77589230E+01 4
C6H11O2r_R5_2 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
1
-4.78339911E-01 6.93274446E-02-2.29500282E-05-1.95859735E-08 1.30240931E-11 2

-2.45543682E+03 3.39794984E+01-4.78339911E-01 6.93274446E-02-2.29500282E-
 05 3
 -1.95859735E-08 1.30240931E-11-2.45543682E+03 3.39794984E+01
 4
 C5H7Or_R5 C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 -2.06085731E+00 5.05345705E-02-2.35149128E-05 2.48923420E-10 1.79780657E-
 12 2
 1.06505219E+04 3.60070425E+01-2.06085731E+00 5.05345705E-02-2.35149128E-
 05 3
 2.48923420E-10 1.79780657E-12 1.06505219E+04 3.60070425E+01
 4
 C6H7O2r_R5_2 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 -7.77488958E+00 1.24263305E-01-2.00477995E-04 1.78525865E-07-6.29393369E-
 11 2
 1.97155289E+04 5.93273390E+01-7.77488958E+00 1.24263305E-01-2.00477995E-
 04 3
 1.78525865E-07-6.29393369E-11 1.97155289E+04 5.93273390E+01
 4
 Ccy(CCC*CC) C 6 H 10 G 3E+02 2E+03 1E+03
 1
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 12 2
 -1.79537671E+02 3.89190505E+01-2.75619093E+00 5.73814188E-02-1.99726315E-
 05 3
 -7.07251219E-09 4.75465846E-12-1.79537671E+02 3.89190505E+01
 4
 C5H8O2_R5 C 5 O 2 H 8 G 3E+02 2E+03 1E+03
 1
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 11 2
 -7.98799340E+03 4.04327994E+01-2.79449890E+00 7.31816512E-02-7.37889609E-
 05 3
 5.36871483E-08-1.92781496E-11-7.98799340E+03 4.04327994E+01
 4
 C(OOJ)cy(CCCCC) C 6 H 11 O 2 G100.000 5000.000 852.45
 1
 1.24306233E+01 3.23687997E-02-2.03216791E-06-4.04301842E-09 4.60684015E-
 13 2
 -1.05888919E+04-3.26926787E+01 2.01791056E+00 3.46877800E-02 7.57828190E-
 05 3
 -1.28946231E-07 5.58746492E-11-7.12262364E+03 2.57988522E+01
 4
 C6H7O2r_Olef_6 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 2.54870950E+00 3.47671154E-02 1.84543344E-05-4.94953868E-08 2.20891592E-
 11 2
 1.79698774E+04 3.48603991E+01 2.54870950E+00 3.47671154E-02 1.84543344E-
 05 3
 -4.94953868E-08 2.20891592E-11 1.79698774E+04 3.48603991E+01
 4
 C6H12O3_Olef C 6 O 3 H 12 G 3E+02 2E+03 1E+03
 1
 6.36360217E-01 1.05795511E-01-1.17152758E-04 7.62331341E-08-2.17386467E-
 11 2
 -4.03689493E+04 2.65208563E+01 6.36360217E-01 1.05795511E-01-1.17152758E-
 04 3

7.62331341E-08-2.17386467E-11-4.03689493E+04 2.65208563E+01
 4
 C6H9O2r_R5 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 -6.47404797E+00 1.15678242E-01-1.62483630E-04 1.35858303E-07-4.70741689E-11 2
 6.43712562E+03 5.32784238E+01-6.47404797E+00 1.15678242E-01-1.62483630E-04 3
 1.35858303E-07-4.70741689E-11 6.43712562E+03 5.32784238E+01
 4
 CC(OH)CC*CCOJ C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 6.91912266E+00 4.42938129E-02 1.62692449E-06-2.59090262E-08 1.16947181E-11 2
 -2.14212378E+04 2.07524655E+00 6.91912266E+00 4.42938129E-02 1.62692449E-06 3
 -2.59090262E-08 1.16947181E-11-2.14212378E+04 2.07524655E+00
 4
 C6H12O2_Olef_1 C 6 O 2 H 12 G 3E+02 2E+03 1E+03
 1
 3.64371768E+00 7.30443666E-02-6.04593885E-05 3.54542890E-08-1.10148673E-11 2
 -1.84952659E+04 1.47365250E+01 3.64371768E+00 7.30443666E-02-6.04593885E-05 3
 3.54542890E-08-1.10148673E-11-1.84952659E+04 1.47365250E+01
 4
 JOOcy(CCC*CCC) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 -3.76169839E+00 9.34737550E-02-1.06080717E-04 7.92081496E-08-2.69446707E-11 2
 5.07205774E+03 4.30081174E+01-3.76169839E+00 9.34737550E-02-1.06080717E-04 3
 7.92081496E-08-2.69446707E-11 5.07205774E+03 4.30081174E+01
 4
 C4H8O2 C 4 O 2 H 8 G 3E+02 2E+03 1E+03
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 5.65405953E+00 2.54662123E-02 2.36326203E-05-4.63089420E-08 1.96819202E-11 2
 -4.84218166E+04 4.87625695E+00 5.65405953E+00 2.54662123E-02 2.36326203E-05 3
 -4.63089420E-08 1.96819202E-11-4.84218166E+04 4.87625695E+00
 4
 COOJcy(CCC*CC) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 7.87918680E+03 4.38381609E+01-3.07996589E+00 8.81316841E-02-1.05693272E-04 3
 8.73913390E-08-3.18861127E-11 7.87918680E+03 4.38381609E+01
 4
 C6H9O2r_R6_1 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 -4.98842633E+00 1.11516553E-01-1.42901147E-04 1.09916581E-07-3.65249178E-11 2
 1.03123965E+04 4.66007457E+01-4.98842633E+00 1.11516553E-01-1.42901147E-04 3
 1.09916581E-07-3.65249178E-11 1.03123965E+04 4.66007457E+01
 4

CPcy(CCJC*CC) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 5.95585792E+03 4.30035542E+01-3.33056291E+00 8.99791634E-02-9.91904203E-05 3
 7.44597825E-08-2.60145395E-11 5.95585792E+03 4.30035542E+01
 4
 C*cy(CCCCC) C 6 H 10 G 3E+02 2E+03 1E+03
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 -2.55974725E+02 3.44785302E+01-1.86040052E+00 4.47279586E-02 2.92814729E-05 3
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 4
 C6H10_R5 C 6 H 10 G 3E+02 2E+03 1E+03
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 -3.99144444E+02 2.70423006E+01-2.83915111E-01 4.55598127E-02 4.84138960E-06 3
 -3.07297516E-08 1.30615326E-11-3.99144444E+02 2.70423006E+01
 4
 C6H7O2r_R5 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
 1
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 1.97155289E+04 5.93273390E+01-7.77488958E+00 1.24263305E-01-2.00477995E-04 3
 1.78525865E-07-6.29393369E-11 1.97155289E+04 5.93273390E+01
 4
 C6H11O2r_4 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 -2.26398494E+04 8.34214212E+00 4.82602109E+00 6.10899954E-02-2.76630054E-05 3
 -5.42645054E-09 6.54834471E-12-2.26398494E+04 8.34214212E+00
 4
 C*CCJCC*O C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 1.38714297E+00 4.54590269E-02-1.84267439E-05-8.29704954E-09 6.93182004E-12 2
 2.71465633E+03 2.27702079E+01 1.38714297E+00 4.54590269E-02-1.84267439E-05 3
 -8.29704954E-09 6.93182004E-12 2.71465633E+03 2.27702079E+01
 4
 C6H11O2r_R5_11 C 6 H 11 O 2 G100.000 5000.000 856.69
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 1.24574259E+01 3.36468020E-02-3.24479693E-06-3.80602445E-09 4.44596929E-13 2
 -5.51348849E+03-3.11160823E+01 1.96677739E+00 3.54714289E-02 7.61299894E-05 3
 -1.29829428E-07 5.59717790E-11-1.98555399E+03 2.79724036E+01
 4
 C6H11O2r_R5_8 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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-5.17093541E-01 7.19322023E-02-3.82721978E-05 1.47074859E-09 4.31156476E-
 12 2
 -8.22977040E+03 3.12213440E+01-5.17093541E-01 7.19322023E-02-3.82721978E-
 05 3
 1.47074859E-09 4.31156476E-12-8.22977040E+03 3.12213440E+01
 4
 C*CC(OJ)CCC C 6 O 1 H 11 G 3E+02 2E+03 1E+03
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 11 2
 -1.98477743E+03 2.82470637E+00 5.74027698E+00 4.51350339E-02-2.59566063E-
 07 3
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 4
 C6H7O2r_Olef_2 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
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 11 2
 1.79679082E+04 2.14958749E+01-2.87966431E+00 1.02727277E-01-1.30162978E-
 04 3
 9.01645809E-08-2.62139081E-11 1.79679082E+04 2.14958749E+01
 4
 C6H10O_Olef C 6 O 1 H 10 G 3E+02 2E+03 1E+03
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 4.55950250E-08-1.43720309E-11-2.39256909E+04 1.61392313E+01
 4
 C6H9O2r_R5_1 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 11 2
 6.21751885E+03 4.14016739E+01-4.00177215E+00 1.03856636E-01-1.37669609E-
 04 3
 1.12201063E-07-3.87672948E-11 6.21751885E+03 4.14016739E+01
 4
 HOOcy(CCC*CCJC) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 11 2
 3.14872886E+03 4.21735106E+01-4.01229540E+00 9.53212343E-02-9.95778652E-
 05 3
 6.62765931E-08-2.10730974E-11 3.14872886E+03 4.21735106E+01
 4
 C6H7O2r_Olef_5 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
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 11 2
 1.82280365E+04 3.05704847E+01-1.66825249E+00 8.93223773E-02-1.09579859E-
 04 3
 7.60663503E-08-2.21423273E-11 1.82280365E+04 3.05704847E+01
 4
 C5H9Or_Olef C 5 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 2.57448528E+00 4.91185201E-02-2.05113654E-05-8.72978609E-09 7.73908041E-
 12 2

4.53364461E+03 1.71660193E+01 2.57448528E+00 4.91185201E-02-2.05113654E-
05 3
-8.72978609E-09 7.73908041E-12 4.53364461E+03 1.71660193E+01
4
C6H7O2r_Olef_4 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
1
-3.11920162E+00 9.16135315E-02-9.22050141E-05 4.45692987E-08-7.79814061E-
12 2
1.82923952E+04 3.59578078E+01-3.11920162E+00 9.16135315E-02-9.22050141E-
05 3
4.45692987E-08-7.79814061E-12 1.82923952E+04 3.59578078E+01
4
CCCC*CCOJ C 6 O 1 H 11 G 3E+02 2E+03 1E+03
1
7.83337855E+00 2.83388514E-02 2.90303639E-05-4.62052956E-08 1.72721241E-
11 2
-7.66165889E+02-3.44218921E+00 7.83337855E+00 2.83388514E-02 2.90303639E-
05 3
-4.62052956E-08 1.72721241E-11-7.66165889E+02-3.44218921E+00
4
C6H9O2r_R6 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
1
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11 2
4.89639955E+03 4.56500630E+01-5.18292017E+00 1.13033582E-01-1.52383669E-
04 3
1.22797400E-07-4.17093486E-11 4.89639955E+03 4.56500630E+01
4
C6H9O2r_R5_2 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
1
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11 2
3.26885422E+03 4.05872966E+01-2.59670782E+00 7.86577846E-02-7.53685620E-
05 3
5.43941740E-08-1.98483552E-11 3.26885422E+03 4.05872966E+01
4
C6H7O2r_Olef C 6 O 2 H 7 G 3E+02 2E+03 1E+03
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11 2
1.99909400E+04 2.44843080E+01 6.05576473E-01 7.52354642E-02-8.61970339E-
05 3
6.01268956E-08-1.82032268E-11 1.99909400E+04 2.44843080E+01
4
C6H11O2r_R5_7 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
1
1.03286993E+00 5.64133419E-02 5.04895515E-06-4.44934238E-08 2.11117824E-
11 2
-3.65257729E+03 2.87526533E+01 1.03286993E+00 5.64133419E-02 5.04895515E-
06 3
-4.44934238E-08 2.11117824E-11-3.65257729E+03 2.87526533E+01
4
C6H9O2r_R5_4 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
1
-6.72464498E+00 1.17525721E-01-1.55980778E-04 1.22926746E-07-4.12025957E-
11 2
4.51379674E+03 5.31369642E+01-6.72464498E+00 1.17525721E-01-1.55980778E-
04 3

1.22926746E-07-4.12025957E-11 4.51379674E+03 5.31369642E+01
 4
 C6H7O2r_Olef_7 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 -8.45372653E-01 7.75266184E-02-6.88221892E-05 2.86298440E-08-3.85904007E-
 12 2
 2.00552987E+04 2.98716311E+01-8.45372653E-01 7.75266184E-02-6.88221892E-
 05 3
 2.86298440E-08-3.85904007E-12 2.00552987E+04 2.98716311E+01
 4
 C6H7O2r_R5_1 C 6 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 -3.82718554E+00 1.01243585E-01-1.49961695E-04 1.30742082E-07-4.64999472E-
 11 2
 2.16544515E+04 4.12871936E+01-3.82718554E+00 1.01243585E-01-1.49961695E-
 04 3
 1.30742082E-07-4.64999472E-11 2.16544515E+04 4.12871936E+01
 4
 C6H10O2_Olef_3 C 6 O 2 H 10 G 3E+02 2E+03 1E+03
 1
 1.73804445E+00 8.50025575E-02-9.46802765E-05 6.58912944E-08-1.99494369E-
 11 2
 -4.45807628E+04 2.16566671E+01 1.73804445E+00 8.50025575E-02-9.46802765E-
 05 3
 6.58912944E-08-1.99494369E-11-4.45807628E+04 2.16566671E+01
 4
 C4H7O2r_Olef_3 C 4 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 2.15974804E-01 7.10271737E-02-9.25625205E-05 7.21021674E-08-2.39291909E-
 11 2
 1.02199614E+04 2.77974224E+01 2.15974804E-01 7.10271737E-02-9.25625205E-
 05 3
 7.21021674E-08-2.39291909E-11 1.02199614E+04 2.77974224E+01
 4
 C6H11O2r_4 (m3) C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 2.77850102E+00 6.84253383E-02-4.33887492E-05 1.29199959E-08-1.62077554E-
 12 2
 -4.36572713E+03 1.76262280E+01 2.77850102E+00 6.84253383E-02-4.33887492E-
 05 3
 1.29199959E-08-1.62077554E-12-4.36572713E+03 1.76262280E+01
 4
 C5H8O3_Olef_1 C 5 O 3 H 8 G 3E+02 2E+03 1E+03
 1
 2.32763786E+00 7.54468964E-02-9.13408009E-05 7.14693369E-08-2.44742906E-
 11 2
 -2.49741993E+04 2.08874918E+01 2.32763786E+00 7.54468964E-02-9.13408009E-
 05 3
 7.14693369E-08-2.44742906E-11-2.49741993E+04 2.08874918E+01
 4
 C6H10O_Olef_12 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
 1
 8.23280722E+00 1.65650194E-02 8.15357248E-05-1.18789136E-07 4.82528627E-
 11 2
 -8.11301806E+03-1.12336502E+01 8.23280722E+00 1.65650194E-02 8.15357248E-
 05 3
 -1.18789136E-07 4.82528627E-11-8.11301806E+03-1.12336502E+01
 4

C5H7Or_Olef_4 C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 -1.33076044E+00 8.21143283E-02-1.16862786E-04 9.63808762E-08-3.21185910E-
 11 2
 6.70987839E+03 3.05712166E+01-1.33076044E+00 8.21143283E-02-1.16862786E-
 04 3
 9.63808762E-08-3.21185910E-11 6.70987839E+03 3.05712166E+01
 4
 C6H11O3r_10 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 5.57257389E+00 6.84727094E-02-5.64379549E-05 3.66264177E-08-1.29535327E-
 11 2
 -1.22781522E+04 8.29803654E+00 5.57257389E+00 6.84727094E-02-5.64379549E-
 05 3
 3.66264177E-08-1.29535327E-11-1.22781522E+04 8.29803654E+00
 4
 C6H10O3_Olef_18 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
 1
 2.36435597E+00 1.01194723E-01-1.42257750E-04 1.23549025E-07-4.41743093E-
 11 2
 -3.41712742E+04 1.99825275E+01 2.36435597E+00 1.01194723E-01-1.42257750E-
 04 3
 1.23549025E-07-4.41743093E-11-3.41712742E+04 1.99825275E+01
 4
 C6H11O3r_7 (m5) C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 3.47947232E+00 8.52688920E-02-8.57278849E-05 5.71089933E-08-1.80999060E-
 11 2
 -1.34967637E+04 1.45649321E+01 3.47947232E+00 8.52688920E-02-8.57278849E-
 05 3
 5.71089933E-08-1.80999060E-11-1.34967637E+04 1.45649321E+01
 4
 C6H9O2r_Olef_7 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 5.25303634E+00 6.72395827E-02-8.02684253E-05 6.98738287E-08-2.59290008E-
 11 2
 -1.66656239E+04 6.07579285E+00 5.25303634E+00 6.72395827E-02-8.02684253E-
 05 3
 6.98738287E-08-2.59290008E-11-1.66656239E+04 6.07579285E+00
 4
 C5H9O2r_Olef_1 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 1.22793652E+00 7.32974167E-02-7.85762449E-05 5.38056578E-08-1.69091703E-
 11 2
 1.36767302E+04 2.33888092E+01 1.22793652E+00 7.32974167E-02-7.85762449E-
 05 3
 5.38056578E-08-1.69091703E-11 1.36767302E+04 2.33888092E+01
 4
 C6H10O3_Olef_10 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
 1
 -5.89636868E+00 1.44484959E-01-2.24906505E-04 1.93561837E-07-6.63676748E-
 11 2
 -3.44932833E+04 5.64767437E+01-5.89636868E+00 1.44484959E-01-2.24906505E-
 04 3
 1.93561837E-07-6.63676748E-11-3.44932833E+04 5.64767437E+01
 4
 C6H11O2r_16 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1

1.51478552E+00 8.84436876E-02-1.00489046E-04 7.24467154E-08-2.29997333E-
 11 2
 -1.40956962E+03 2.09806225E+01 1.51478552E+00 8.84436876E-02-1.00489046E-
 04 3
 7.24467154E-08-2.29997333E-11-1.40956962E+03 2.09806225E+01
 4
 C5H7O2r_Olef_1 C 5 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 6.51729873E+00 3.07413812E-02-1.85104844E-06-1.01902477E-08 3.81270077E-
 12 2
 -7.24509934E+03 3.80738989E+00 6.51729873E+00 3.07413812E-02-1.85104844E-
 06 3
 -1.01902477E-08 3.81270077E-12-7.24509934E+03 3.80738989E+00
 4
 C6H11O3r_40 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 7.54543418E+00 6.04859782E-02-4.59505494E-05 3.17487048E-08-1.25301544E-
 11 2
 -1.10117492E+04 1.49971927E+00 7.54543418E+00 6.04859782E-02-4.59505494E-
 05 3
 3.17487048E-08-1.25301544E-11-1.10117492E+04 1.49971927E+00
 4
 C6H11O2r_9 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 2.93600730E+00 6.88838611E-02-5.41860944E-05 2.88574647E-08-8.23505535E-
 12 2
 -1.23391143E+03 1.83386769E+01 2.93600730E+00 6.88838611E-02-5.41860944E-
 05 3
 2.88574647E-08-8.23505535E-12-1.23391143E+03 1.83386769E+01
 4
 C6H11O2r_13 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 4.45255992E+00 6.19680814E-02-3.41472992E-05 6.23762571E-09 3.13938412E-
 13 2
 4.41296146E+03 1.33522649E+01 4.45255992E+00 6.19680814E-02-3.41472992E-
 05 3
 6.23762571E-09 3.13938412E-13 4.41296146E+03 1.33522649E+01
 4
 C5H7Or_Olef (m6) C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 9.08398962E-01 7.20642899E-02-1.02406715E-04 8.70530688E-08-2.98846385E-
 11 2
 9.28925854E+03 2.11665656E+01 9.08398962E-01 7.20642899E-02-1.02406715E-
 04 3
 8.70530688E-08-2.98846385E-11 9.28925854E+03 2.11665656E+01
 4
 C5H9O2r_Olef_2 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 -1.93285268E-01 9.28572431E-02-1.24879197E-04 9.73949085E-08-3.16738483E-
 11 2
 1.35010720E+04 2.60307548E+01-1.93285268E-01 9.28572431E-02-1.24879197E-
 04 3
 9.73949085E-08-3.16738483E-11 1.35010720E+04 2.60307548E+01
 4
 C6H9O2r_Olef_14 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 4.19694260E+00 6.28905520E-02-5.32379369E-05 3.28488283E-08-1.03799797E-
 11 2

-1.51975913E+04 1.23086130E+01 4.19694260E+00 6.28905520E-02-5.32379369E-
 05 3
 3.28488283E-08-1.03799797E-11-1.51975913E+04 1.23086130E+01
 4
 C6H13O4r_1 C 6 O 4 H 13 G 3E+02 2E+03 1E+03
 1
 5.12161373E+00 9.26361082E-02-1.02481388E-04 8.08653405E-08-2.92075761E-
 11 2
 -2.73308853E+04 1.04920213E+01 5.12161373E+00 9.26361082E-02-1.02481388E-
 04 3
 8.08653405E-08-2.92075761E-11-2.73308853E+04 1.04920213E+01
 4
 C4H5Or_Olef C 4 O 1 H 5 G 3E+02 2E+03 1E+03
 1
 2.46753022E+00 3.25820872E-02-1.62741481E-05-1.22675942E-09 2.94204076E-
 12 2
 1.89500617E+04 1.79876730E+01 2.46753022E+00 3.25820872E-02-1.62741481E-
 05 3
 -1.22675942E-09 2.94204076E-12 1.89500617E+04 1.79876730E+01
 4
 C*CC(OOH)C*C C 5 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 -1.00718706E-01 8.37108139E-02-1.05318323E-04 7.78960632E-08-2.46604588E-
 11 2
 -4.87203263E+02 2.64673373E+01-1.00718706E-01 8.37108139E-02-1.05318323E-
 04 3
 7.78960632E-08-2.46604588E-11-4.87203263E+02 2.64673373E+01
 4
 C6H11O3r_38 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 3.54217045E+00 8.46270078E-02-8.95643165E-05 6.52825549E-08-2.21044771E-
 11 2
 -1.29429507E+04 1.55719707E+01 3.54217045E+00 8.46270078E-02-8.95643165E-
 05 3
 6.52825549E-08-2.21044771E-11-1.29429507E+04 1.55719707E+01
 4
 C3H7O2r_2 C 3 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 1.71381925E+00 4.73028061E-02-3.36502562E-05 7.18703046E-09 1.86686069E-
 12 2
 -2.00212830E+03 1.93250228E+01 1.71381925E+00 4.73028061E-02-3.36502562E-
 05 3
 7.18703046E-09 1.86686069E-12-2.00212830E+03 1.93250228E+01
 4
 C6H11O2r_23 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 7.01999105E-01 9.58756852E-02-1.08098216E-04 7.28137815E-08-2.15764489E-
 11 2
 5.52703523E+03 2.53832615E+01 7.01999105E-01 9.58756852E-02-1.08098216E-
 04 3
 7.28137815E-08-2.15764489E-11 5.52703523E+03 2.53832615E+01
 4
 C6H10O3_Olef_7 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
 1
 1.06337547E+00 1.11945098E-01-1.69758178E-04 1.51533413E-07-5.42159922E-
 11 2
 -3.43947239E+04 2.42545071E+01 1.06337547E+00 1.11945098E-01-1.69758178E-
 04 3

1.51533413E-07-5.42159922E-11-3.43947239E+04 2.42545071E+01
 4
 C3H5O2r_Olef_1 C 3 O 2 H 5 G 3E+02 2E+03 1E+03
 1
 1.41833408E+00 3.63206077E-02-7.27011920E-06-2.31441598E-08 1.38795166E-11 2
 4.31360251E+03 2.17666013E+01 1.41833408E+00 3.63206077E-02-7.27011920E-06 3
 -2.31441598E-08 1.38795166E-11 4.31360251E+03 2.17666013E+01
 4
 C5H8O2_Olef C 5 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 3.72561115E+00 5.28615829E-02-4.41821129E-05 2.83480579E-08-9.85051712E-12 2
 3.73200476E+03 1.45365521E+01 3.72561115E+00 5.28615829E-02-4.41821129E-05 3
 2.83480579E-08-9.85051712E-12 3.73200476E+03 1.45365521E+01
 4
 C6H11O3r_23 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 2.34530469E-02 1.07327326E-01-1.24943589E-04 8.53303531E-08-2.53109412E-11 2
 -1.25873484E+04 2.79124243E+01 2.34530469E-02 1.07327326E-01-1.24943589E-04 3
 8.53303531E-08-2.53109412E-11-1.25873484E+04 2.79124243E+01
 4
 C6H13O4r_6 C 6 O 4 H 13 G 3E+02 2E+03 1E+03
 1
 3.14875344E+00 1.00622839E-01-1.12968793E-04 8.57430533E-08-2.96309544E-11 2
 -2.85972883E+04 1.72903386E+01 3.14875344E+00 1.00622839E-01-1.12968793E-04 3
 8.57430533E-08-2.96309544E-11-2.85972883E+04 1.72903386E+01
 4
 C4H4O2_Olef_1 C 4 O 2 H 4 G 3E+02 2E+03 1E+03
 1
 -9.16486313E+00 1.37497733E-01-2.65350784E-04 2.48684768E-07-8.74305270E-11 2
 -2.73194085E+04 5.94237265E+01-9.16486313E+00 1.37497733E-01-2.65350784E-04 3
 2.48684768E-07-8.74305270E-11-2.73194085E+04 5.94237265E+01
 4
 C5H6O2_Olef_1 C 5 O 2 H 6 G 3E+02 2E+03 1E+03
 1
 -2.60151847E+00 9.19330134E-02-1.36346776E-04 1.14064629E-07-3.82204866E-11 2
 -2.76378573E+04 3.83924541E+01-2.60151847E+00 9.19330134E-02-1.36346776E-04 3
 1.14064629E-07-3.82204866E-11-2.76378573E+04 3.83924541E+01
 4
 C6H11O2r_22 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 1.70927936E+00 8.69266589E-02-9.10065245E-05 5.95658956E-08-1.78153025E-11 2
 4.00642732E+03 2.19313053E+01 1.70927936E+00 8.69266589E-02-9.10065245E-05 3
 5.95658956E-08-1.78153025E-11 4.00642732E+03 2.19313053E+01
 4

C4H6O3_Olef_3 C 4 O 3 H 6 G 3E+02 2E+03 1E+03
 1
 5.21504837E+00 4.73984566E-02-5.03200969E-05 3.88156643E-08-1.41052150E-
 11 2
 -2.13652066E+04 6.14394017E+00 5.21504837E+00 4.73984566E-02-5.03200969E-
 05 3
 3.88156643E-08-1.41052150E-11-2.13652066E+04 6.14394017E+00
 4
 C6H11O2r_15 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 2.12322089E+00 7.63158587E-02-6.17952643E-05 2.92245309E-08-6.81177099E-
 12 2
 5.70269342E+03 2.27413160E+01 2.12322089E+00 7.63158587E-02-6.17952643E-
 05 3
 2.92245309E-08-6.81177099E-12 5.70269342E+03 2.27413160E+01
 4
 C6H9O2r_Olef_17 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 2.61627785E+00 7.69720952E-02-9.09565241E-05 7.43439973E-08-2.62763503E-
 11 2
 -1.36754072E+04 1.90046815E+01 2.61627785E+00 7.69720952E-02-9.09565241E-
 05 3
 7.43439973E-08-2.62763503E-11-1.36754072E+04 1.90046815E+01
 4
 C6H9O2r_Olef(m1) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 6.55401684E+00 5.64892076E-02-5.27679980E-05 4.18894408E-08-1.58873180E-
 11 2
 -1.64421742E+04 2.90242557E+00 6.55401684E+00 5.64892076E-02-5.27679980E-
 05 3
 4.18894408E-08-1.58873180E-11-1.64421742E+04 2.90242557E+00
 4
 C6H10O_Olef_25 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
 1
 8.19204597E+00-8.21035036E-04 1.39492342E-04-1.85590571E-07 7.46769919E-
 11 2
 -1.70118895E+04-9.08886506E+00 8.19204597E+00-8.21035036E-04 1.39492342E-
 04 3
 -1.85590571E-07 7.46769919E-11-1.70118895E+04-9.08886506E+00
 4
 C6H11O2r_18 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 3.60788709E+00 7.16475051E-02-7.11991162E-05 5.19641397E-08-1.78533599E-
 11 2
 -1.90958086E+02 1.47137270E+01 3.60788709E+00 7.16475051E-02-7.11991162E-
 05 3
 5.19641397E-08-1.78533599E-11-1.90958086E+02 1.47137270E+01
 4
 C6H8O2_Olef_1 C 6 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 -3.86578087E+00 1.28431215E-01-2.14764152E-04 1.94128706E-07-6.79621882E-
 11 2
 -3.70583819E+04 4.17594693E+01-3.86578087E+00 1.28431215E-01-2.14764152E-
 04 3
 1.94128706E-07-6.79621882E-11-3.70583819E+04 4.17594693E+01
 4
 C6H11O3r_43 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1

7.54543418E+00 6.04859782E-02-4.59505494E-05 3.17487048E-08-1.25301544E-
 11 2
 -1.10117492E+04 1.49971927E+00 7.54543418E+00 6.04859782E-02-4.59505494E-
 05 3
 3.17487048E-08-1.25301544E-11-1.10117492E+04 1.49971927E+00
 4
 C6H12O4_Olef_2 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
 1
 1.38291302E+00 1.13178225E-01-1.45927707E-04 1.18286002E-07-4.12405240E-
 11 2
 -3.00072522E+04 2.64767508E+01 1.38291302E+00 1.13178225E-01-1.45927707E-
 04 3
 1.18286002E-07-4.12405240E-11-3.00072522E+04 2.64767508E+01
 4
 C6H11O3r_5(m0) C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 2.34530469E-02 1.07327326E-01-1.24943589E-04 8.53303531E-08-2.53109412E-
 11 2
 -1.25873484E+04 2.79124243E+01 2.34530469E-02 1.07327326E-01-1.24943589E-
 04 3
 8.53303531E-08-2.53109412E-11-1.25873484E+04 2.79124243E+01
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 11 2
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 05 3
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 C6H12O4_Olef_18 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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 11 2
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 04 3
 1.46942139E-07-5.03914685E-11-3.06720507E+04 3.37506850E+01
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 C6H10O_Olef_14 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
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 10 2
 -7.16997741E+03-3.23835239E+01 1.45486874E+01-5.02948369E-02 2.61490313E-
 04 3
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 C4H5Or_Olef_1 C 4 O 1 H 5 G 3E+02 2E+03 1E+03
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 7.62410395E-01 4.07341045E-02-2.44317301E-05 5.74839719E-10 3.69535323E-
 12 2
 6.95664420E+03 2.25965571E+01 7.62410395E-01 4.07341045E-02-2.44317301E-
 05 3
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 4
 C6H12O4_Olef_23 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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 11 2

-2.87408492E+04 1.85798212E+01 3.35577331E+00 1.05191493E-01-1.35440302E-
 04 3
 1.13408289E-07-4.08171457E-11-2.87408492E+04 1.85798212E+01
 4
 C6H11O2r_1(m2) C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 12 2
 -1.23391143E+03 1.83386769E+01 2.93600730E+00 6.88838611E-02-5.41860944E-
 05 3
 2.88574647E-08-8.23505535E-12-1.23391143E+03 1.83386769E+01
 4
 C3H5O2r_Olef C 3 O 2 H 5 G 3E+02 2E+03 1E+03
 1
 7.19146098E+00 1.75432342E-02 8.27617616E-06-2.24217299E-08 1.00978053E-
 11 2
 2.11806723E+04-4.42733785E+00 7.19146098E+00 1.75432342E-02 8.27617616E-
 06 3
 -2.24217299E-08 1.00978053E-11 2.11806723E+04-4.42733785E+00
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 C6H10O3_Olef_2 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
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 3.91495682E-01 1.09181454E-01-1.52745156E-04 1.28426738E-07-4.45976876E-
 11 2
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 04 3
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 4
 C3H4O2 C 3 O 2 H 4 G 3E+02 2E+03 1E+03
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 12 2
 -3.23421713E+04 1.56339583E+01 3.04246139E+00 2.14712006E-02 4.47125208E-
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 4
 C5H9O2r_Olef_7 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
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 11 2
 1.49431332E+04 1.65904920E+01 3.20079681E+00 6.53106855E-02-6.80888393E-
 05 3
 4.89279449E-08-1.64857920E-11 1.49431332E+04 1.65904920E+01
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 C*CC*CCOOH C 5 O 2 H 8 G 3E+02 2E+03 1E+03
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 4
 C6H10O3_Olef_4 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
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 11 2
 -3.26709102E+04 4.39817130E+01-3.54624331E+00 1.29664342E-01-1.90933682E-
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 4
 C6H11O3r_28 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
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 4.15135211E+00 8.80325359E-02-1.02740907E-04 8.02156684E-08-2.77182106E-
 11 2
 -1.24538104E+04 1.09399821E+01 4.15135211E+00 8.80325359E-02-1.02740907E-
 04 3
 8.02156684E-08-2.77182106E-11-1.24538104E+04 1.09399821E+01
 4
 C6H9O2r_Olef(m4) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 11 2
 -1.40323949E+04 3.91504910E+01-2.81260172E+00 1.07017261E-01-1.40659634E-
 04 3
 1.07443070E-07-3.39107638E-11-1.40323949E+04 3.91504910E+01
 4
 C6H10O3_Olef_15 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
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 11 2
 -3.29266913E+04 3.04873272E+01 7.28173344E-03 1.07596067E-01-1.42727689E-
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 4
 C6H11O3r_20 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
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 11 2
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 4
 C6H9O4r_1 C 6 O 4 H 9 G 3E+02 2E+03 1E+03
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 11 2
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 C*CCCCCOOJ C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 12 2
 3.24915543E+01 1.15403597E+01 4.90886759E+00 6.08971299E-02-4.36986889E-
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 2.39797518E-08-7.81167705E-12 3.24915543E+01 1.15403597E+01
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 C4H7O2r_Olef C 4 O 2 H 7 G 3E+02 2E+03 1E+03
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 8.37277964E-08-2.85320245E-11 5.69676324E+03 2.69896652E+01
 4

C6H9O2r_Olef_10 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 11 2
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 C6H11O2r_24 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 11 2
 4.23730327E+03 1.59942104E+01 3.03133813E+00 8.15279079E-02-8.04502509E-
 05 3
 4.98268764E-08-1.44507395E-11 4.23730327E+03 1.59942104E+01
 4
 C3H6O2_Olef_1 C 3 O 2 H 6 G 3E+02 2E+03 1E+03
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 11 2
 -1.00626493E+04 1.08357316E+01 3.85360610E+00 2.83193220E-02-3.12767886E-
 07 3
 -1.97748559E-08 1.01531909E-11-1.00626493E+04 1.08357316E+01
 4
 C5H8O_Olef_1 C 5 O 1 H 8 G 3E+02 2E+03 1E+03
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 04 3
 9.56259715E-08-3.15146911E-11-1.80291157E+04 3.78210456E+01
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 C5H9O2r_Olef_8 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
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 04 3
 9.03901715E-08-2.83300769E-11 8.65684346E+03 3.09628198E+01
 4
 C5H7O2r_Olef_3 C 5 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 6.23815177E+00 3.49300610E-02-4.57010707E-06-1.34740974E-08 6.47985310E-
 12 2
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 06 3
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 4
 C6H11O3r_13 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
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 11 2
 -1.13687369E+04 2.16455287E+01 2.11655462E+00 9.05311439E-02-9.56536592E-
 05 3
 6.48477774E-08-2.01645679E-11-1.13687369E+04 2.16455287E+01
 4
 C5H8O3_Olef_3 C 5 O 3 H 8 G 3E+02 2E+03 1E+03
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 -2.67328069E+04 1.98513861E+01 2.04849090E+00 7.96355762E-02-9.40598595E-
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 6.81854873E-08-2.18071383E-11-2.67328069E+04 1.98513861E+01
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 C4H4O2_Olef_2 C 4 O 2 H 4 G 3E+02 2E+03 1E+03
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 8.34488338E-08-2.86786845E-11-2.51242741E+04 2.75173734E+01
 4
 C6H12O4_Olef_15 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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 04 3
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 C6H10O_Olef_17 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
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 2.20444081E+00 7.11645923E-02-5.28698166E-05 1.65581244E-08-3.10436903E-
 13 2
 -2.00345871E+04-3.18978421E+00 2.20444081E+00 7.11645923E-02-5.28698166E-
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 4
 C6H9O2r_Olef_2 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
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 -1.67991619E+04 2.30482350E+01 1.12513728E+00 8.65343733E-02-1.02471108E-
 04 3
 7.49885134E-08-2.35217315E-11-1.67991619E+04 2.30482350E+01
 4
 C6H9O4r_3 C 6 O 4 H 9 G 3E+02 2E+03 1E+03
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 C*CCJCCCP C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 05 3
 8.04228307E-09-1.19739724E-12-3.09932414E+03 1.08279107E+01
 4
 C5H6O2_Olef_2 C 5 O 2 H 6 G 3E+02 2E+03 1E+03
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 2.39096557E-02 7.73114111E-02-1.07972270E-04 8.88163958E-08-2.98256283E-
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 C6H10O3_Olef_12 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
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 C5H6O_Olef_2 C 5 O 1 H 6 G 3E+02 2E+03 1E+03
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 C6H13O4r_7 C 6 O 4 H 13 G 3E+02 2E+03 1E+03
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 11 2
 -2.73308853E+04 1.04920213E+01 5.12161373E+00 9.26361082E-02-1.02481388E-
 04 3
 8.08653405E-08-2.92075761E-11-2.73308853E+04 1.04920213E+01
 4
 C6H10O_Olef_3 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
 1
 9.65402900E+00-2.99480702E-03 1.27838677E-04-1.62378386E-07 6.30175407E-
 11 2
 -7.93735987E+03-1.38755958E+01 9.65402900E+00-2.99480702E-03 1.27838677E-
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 4
 C6H11O3r_19 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
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 11 2
 -1.24538104E+04 1.09399821E+01 4.15135211E+00 8.80325359E-02-1.02740907E-
 04 3

8.02156684E-08-2.77182106E-11-1.24538104E+04 1.09399821E+01
 4
 C4H7O2r_Olef_1 C 4 O 2 H 7 G 3E+02 2E+03 1E+03
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 04 3
 1.08104506E-07-3.56003004E-11 1.22886243E+04 3.36351360E+01
 4
 C*CCCJCCP C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 5.44848850E+03 1.24910424E+01 5.10336143E+00 5.93801013E-02-3.42161672E-
 05 3
 1.10989321E-08-2.62724623E-12 5.44848850E+03 1.24910424E+01
 4
 C6H11O3r_46 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
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 -1.22303607E+04 7.76661484E+00 5.45233261E+00 7.72821608E-02-7.52404793E-
 05 3
 5.22312805E-08-1.76765277E-11-1.22303607E+04 7.76661484E+00
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 C6H12O4_Olef_4 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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 -3.12258637E+04 3.27436463E+01-7.10188548E-01 1.29974407E-01-1.75217637E-
 04 3
 1.38768578E-07-4.63868974E-11-3.12258637E+04 3.27436463E+01
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 C2H5O2r C 2 O 2 H 5 G 3E+02 2E+03 1E+03
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 8.86609117E+02 1.91606197E+01 1.42301305E+00 3.76482228E-02-3.07578897E-
 05 3
 9.66409661E-09 2.64391624E-13 8.86609117E+02 1.91606197E+01
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 C4H6O3_Olef C 4 O 3 H 6 G 3E+02 2E+03 1E+03
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 -2.46557504E+04 4.26119114E+01-4.23570679E+00 1.21011616E-01-2.20344810E-
 04 3
 2.06089475E-07-7.36843311E-11-2.46557504E+04 4.26119114E+01
 4
 C6H11O3r_47 C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 5.45233261E+00 7.72821608E-02-7.52404793E-05 5.22312805E-08-1.76765277E-
 11 2
 -1.22303607E+04 7.76661484E+00 5.45233261E+00 7.72821608E-02-7.52404793E-
 05 3
 5.22312805E-08-1.76765277E-11-1.22303607E+04 7.76661484E+00
 4

C6H10O3_Olef_17 C 6 O 3 H 10 G 3E+02 2E+03 1E+03
1
-1.57338302E+00 1.21677610E-01-1.80446277E-04 1.56003582E-07-5.45633417E-
11 2
-3.14045072E+04 3.60847835E+01-1.57338302E+00 1.21677610E-01-1.80446277E-
04 3
1.56003582E-07-5.45633417E-11-3.14045072E+04 3.60847835E+01
4
C5H9O2r_Olef_4 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
1
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11 2
-9.89205816E+02 3.01483408E+01-4.27307046E-01 7.90098912E-02-8.07777112E-
05 3
4.96613750E-08-1.40421695E-11-9.89205816E+02 3.01483408E+01
4
C5H7Or_Olef_6 C 5 O 1 H 7 G 3E+02 2E+03 1E+03
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1.13489638E+00 7.04473283E-02-9.67213910E-05 7.94209412E-08-2.65653292E-
11 2
4.62641373E+03 2.06428094E+01 1.13489638E+00 7.04473283E-02-9.67213910E-
05 3
7.94209412E-08-2.65653292E-11 4.62641373E+03 2.06428094E+01
4
C5H9O2r_Olef_5 C 5 O 2 H 9 G 3E+02 2E+03 1E+03
1
3.59839590E+00 6.56282113E-02-7.18568113E-05 5.37855837E-08-1.83723951E-
11 2
9.37353641E+03 1.30662544E+01 3.59839590E+00 6.56282113E-02-7.18568113E-
05 3
5.37855837E-08-1.83723951E-11 9.37353641E+03 1.30662544E+01
4
C5H7Or_Olef_1 C 5 O 1 H 7 G 3E+02 2E+03 1E+03
1
3.51517740E+00 3.54344036E-02 3.18487866E-06-2.79854729E-08 1.32973043E-
11 2
1.61672249E+04 1.32533321E+01 3.51517740E+00 3.54344036E-02 3.18487866E-
06 3
-2.79854729E-08 1.32973043E-11 1.61672249E+04 1.32533321E+01
4
C6H9O2r_Olef_12 C 6 O 2 H 9 G 3E+02 2E+03 1E+03
1
-7.77804228E-01 1.04518653E-01-1.47746881E-04 1.22810961E-07-4.14644066E-
11 2
-1.51174684E+04 2.84449444E+01-7.77804228E-01 1.04518653E-01-1.47746881E-
04 3
1.22810961E-07-4.14644066E-11-1.51174684E+04 2.84449444E+01
4
C6H10O_Olef_(m7) C 6 O 1 H 10 G 3E+02 2E+03 1E+03
1
1.11546053E+01-2.27482792E-02 2.04699955E-04-2.69000475E-07 1.12831883E-
10 2
-8.61203858E+03-2.18446488E+01 1.11546053E+01-2.27482792E-02 2.04699955E-
04 3
-2.69000475E-07 1.12831883E-10-8.61203858E+03-2.18446488E+01
4
C6H12O4_Olef_12 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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-7.10188548E-01 1.29974407E-01-1.75217637E-04 1.38768578E-07-4.63868974E-
 11 2
 -3.12258637E+04 3.27436463E+01-7.10188548E-01 1.29974407E-01-1.75217637E-
 04 3
 1.38768578E-07-4.63868974E-11-3.12258637E+04 3.27436463E+01
 4
 C6H12O4_Olef_20 C 6 O 4 H 12 G 3E+02 2E+03 1E+03
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 1.26267174E+00 1.21987676E-01-1.64730232E-04 1.33890865E-07-4.59635191E-
 11 2
 -2.99594607E+04 2.48467168E+01 1.26267174E+00 1.21987676E-01-1.64730232E-
 04 3
 1.33890865E-07-4.59635191E-11-2.99594607E+04 2.48467168E+01
 4
 C6H11O2r_3 C 6 O 2 H 11 G 3E+02 2E+03 1E+03
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 13 2
 4.41296146E+03 1.33522649E+01 4.45255992E+00 6.19680814E-02-3.41472992E-
 05 3
 6.23762571E-09 3.13938412E-13 4.41296146E+03 1.33522649E+01
 4
 C6H10O_Olef_22 C 6 O 1 H 10 G 3E+02 2E+03 1E+03
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 8.29550535E+00 1.59231353E-02 7.76992932E-05-1.10615574E-07 4.42482917E-
 11 2
 -7.55920503E+03-1.02266116E+01 8.29550535E+00 1.59231353E-02 7.76992932E-
 05 3
 -1.10615574E-07 4.42482917E-11-7.55920503E+03-1.02266116E+01
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 C5H7Or_Olef_3 C 5 H 7 O 1 G100.000 5000.000 1925.33
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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
 C*CC*CCC*O C 6 H 8 O 1 G100.000 5000.000 1953.03
 1
 -7.85026052E+01 1.45820830E-01-5.00308491E-05 1.05422518E-09 2.75341293E-
 13 2
 4.08700372E+04 4.97540225E+02-2.39176980E-01 6.39000077E-02-4.73040609E-
 05 3
 2.06697924E-08-4.86563544E-12-4.64665245E+03 2.93113251E+01
 4
 C6H11Or_Olef_39 C 6 H 11 O 1 G100.000 5000.000 737.74
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 3.75349770E+00 5.40593476E-02-2.57865229E-05 4.66026331E-09-3.06473637E-
 13 2
 -1.10689610E+04 1.28239655E+01 1.72027568E+00 4.54956571E-02 3.14521974E-
 05 3
 -8.30541219E-08 4.16136315E-11-1.02359239E+04 2.56273117E+01
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 C6H11Or_Olef_5 C 6 H 11 O 1 G100.000 5000.000 1105.34
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 1.34408848E+01 3.44902064E-02-1.35809251E-05 2.48842667E-09-1.72891049E-
 13 2

-1.65769590E+04-4.07229566E+01 8.41644826E-01 6.01152011E-02-2.12561349E-
 05 3
 -9.22686805E-09 6.17353636E-12-1.25717883E+04 2.68410879E+01
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 CPC*CCJC*C C 6 H 9 O 2 G100.000 5000.000 875.20
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 1.17548951E+01 3.83527311E-02-1.61741088E-05 2.91261937E-09-1.96095526E-
 13 2
 4.37115700E+03-2.77334842E+01 5.33446870E-01 6.81522188E-02-3.04210444E-
 05 3
 -1.42867669E-08 1.27298494E-11 7.15827701E+03 2.96089825E+01
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 13 2
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 05 3
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 14 2
 1.42382219E+04 1.37254549E+02 1.39479327E-01 6.06761189E-02-5.67993499E-
 05 3
 2.71972025E-08-5.25634414E-12 1.33232702E+03 2.59484127E+01
 4
 C6H11Or_olef_46 C 6 H 11 O 1 G100.000 5000.000 1056.74
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 1.41760884E+01 3.38120640E-02-1.33657115E-05 2.47009747E-09-1.73194077E-
 13 2
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 05 3
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 4
 C6H11Or_olef_44 C 6 H 11 O 1 G100.000 5000.000 1240.20
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 13 2
 -6.58470495E+03-4.42653947E+01 2.88730722E+00 5.23749034E-02-1.54818157E-
 05 3
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 4
 JOOcy(CCCCC) C 6H 11O 2 G 0300.00 5000.00 1000.00
 1
 0.20162477E+02 0.29791869E-01-0.97306547E-05 0.15115423E-08-0.91580186E-
 13 2
 -0.19940488E+05-0.84555893E+02-0.21456919E+01 0.66352427E-01 0.24983692E-
 05 3
 -0.45027374E-07 0.20026791E-10-0.12377884E+05 0.37351788E+02
 4
 HOOcy(CCCJCCC) C 6H 11O 2 G 0300.00 5000.00 1000.00
 1
 0.21005251E+02 0.28179143E-01-0.89765790E-05 0.13700221E-08-0.82013850E-
 13 2
 -0.14325531E+05-0.85189323E+02-0.65244335E+00 0.63498124E-01 0.31467200E-
 05 3

-0.43772484E-07 0.19340845E-10-0.69673730E+04 0.33227894E+02
 4
 HOOcy (CCJCCCC) C 6H 110 2 G 0300.00 5000.00 1000.00
 1
 0.21005251E+02 0.28179143E-01-0.89765790E-05 0.13700221E-08-0.82013850E-
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 -0.14325531E+05-0.85189323E+02-0.65244335E+00 0.63498124E-01 0.31467200E-
 05 3
 -0.43772484E-07 0.19340845E-10-0.69673730E+04 0.33227894E+02
 4
 HOOcy (CCCCJCC) C 6H 110 2 G 0300.00 5000.00 1000.00
 1
 2.19171837E+01 2.63008887E-02-8.70871777E-06 1.32408606E-09-7.57493614E-
 14 2
 -1.31159545E+04-9.31104597E+01-3.64623795E+00 8.87056624E-02-6.67784829E-
 05 3
 2.57718948E-08-3.99837603E-12-4.62966929E+03 4.30241674E+01
 4
 HOOcy (CJCCCCC) C 6H 110 2 G 0300.00 5000.00 1000.00
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 0.20648170E+02 0.28225712E-01-0.89463738E-05 0.13619339E-08-0.81458820E-
 13 2
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 05 3
 -0.34969247E-07 0.16273110E-10-0.87683809E+04 0.33516243E+02
 4
 O*cy (CCCCC) C 6H 100 1 G 0300.00 5000.00 1000.00
 1
 0.11009619E+02 0.38478710E-01-0.15103216E-04 0.26677678E-08-0.17660224E-
 12 2
 -0.34532844E+05-0.39168152E+02-0.70734839E+01 0.81469052E-01-0.51488671E-
 04 3
 0.16908398E-07-0.29927343E-11-0.28813357E+05 0.56905037E+02
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 epoxy14cy6 C 6H 100 1 G 0300.00 5000.00 1000.00
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 1.75324245E+01 2.64817085E-02-9.08894671E-06 1.41461033E-09-8.22234020E-
 14 2
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 epoxy12cy6 C 6H 100 1 G 0300.00 5000.00 1000.00
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 1.75470247E+01 2.65395275E-02-9.12476634E-06 1.42188066E-09-8.27154560E-
 14 2
 -2.49198640E+04-7.56242897E+01-7.22057622E+00 8.43843635E-02-6.05934773E-
 05 3
 2.21977283E-08-3.29535043E-12-1.63538964E+04 5.73368598E+01
 4
 C*CC*CCCJ*O C 6 H 7 O 1 G100.000 5000.000 1898.73
 1
 -7.28229027E+01 1.40437384E-01-5.13918328E-05 2.30071859E-09 1.64617039E-
 13 2
 5.50643763E+04 4.62661036E+02 1.24591989E-02 6.16367511E-02-4.81044529E-
 05 3
 2.18498465E-08-5.13530151E-12 1.39509839E+04 2.91414471E+01
 4

Ccy(C(C)C*CC*C) C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -2.05394057E+00 5.83326753E-02 2.38945262E-05-8.56739305E-08 4.20831833E-
 11 2
 8.55872544E+03 3.24747774E+01-2.05394057E+00 5.83326753E-02 2.38945262E-
 05 3
 -8.56739305E-08 4.20831833E-11 8.55872544E+03 3.24747774E+01
 4
 C*CCcyCJC*CC*C C 8 H 9 G 3E+02 2E+03 1E+03
 1
 3.17212932E+00 5.67684514E-02 4.96632550E-06-5.18495830E-08 2.62853540E-
 11 2
 3.16996205E+04-3.89391737E+00 3.17212932E+00 5.67684514E-02 4.96632550E-
 06 3
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 4
 C*CCJcyCC*CC*C C 8 H 9 G 3E+02 2E+03 1E+03
 1
 4.17564974E-01 5.07637761E-02 3.66485233E-05-9.55614415E-08 4.49900243E-
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 C*CC*cyCCJC*CC C 8 H 9 G 3E+02 2E+03 1E+03
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 1.00231751E+00 5.19765042E-02 3.12321193E-05-8.67853286E-08 4.10800485E-
 11 2
 3.23074389E+04 2.24844310E+01 1.00231751E+00 5.19765042E-02 3.12321193E-
 05 3
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 4
 C*CC*cyCCJCC*C C 8 H 9 G 3E+02 2E+03 1E+03
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 13 2
 3.44591262E+04 5.16315559E+01-5.37813770E+00 8.65141646E-02-5.80534051E-
 05 3
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 bicyclicC8H9 C 8 H 9 G100.000 5000.000 893.07
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 13 2
 1.93288230E+04-8.66055653E+01 9.50508969E-02 5.18024076E-02 4.17274789E-
 05 3
 -1.01940280E-07 4.66481810E-11 2.39553519E+04-5.92313777E+00
 4
 C*CCcyCC*CC*C C 8 H 10 G 3E+02 2E+03 1E+03
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 05 3
 -7.92403831E-08 3.98206980E-11 2.20570256E+04 3.25818685E+01
 4
 C6H5C2H3 C 8 H 8 G 3E+02 2E+03 1E+03
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-6.62043000E+00 8.97300000E-02-7.62100000E-05 3.28600000E-08-5.61300000E-
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 1.64800000E+04 5.56000000E+01-6.62043000E+00 8.97300000E-02-7.62100000E-
 05 3
 3.28600000E-08-5.61300000E-12 1.64800000E+04 5.56000000E+01
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 C*CCcy(C*CC*CC) C 8 H 10 G 3E+02 2E+03 1E+03
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 11 2
 2.06804885E+04 1.68208683E+01 2.39896211E+00 4.37516404E-02 5.29763398E-
 05 3
 -1.09999883E-07 4.96925640E-11 2.06804885E+04 1.68208683E+01
 4
 C*CCcy(C*CCC*C) C 8 H 10 G 3E+02 2E+03 1E+03
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 05 3
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 13 2
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 05 3
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 C10H8 C 10 H 8 G 3E+02 2E+03 1E+03
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 1.68018074E+04 5.53768411E+01-7.06891810E+00 9.05551245E-02-4.45142465E-
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 C10H9 C 10 H 9 G 3E+02 2E+03 1E+03
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 C6H5C*CC*CJ C 10 H 9 G 3E+02 2E+03 1E+03
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 11 2
 5.51442883E+04 4.94977536E+01-4.69226525E+00 9.30731095E-02-5.38062685E-
 05 3
 -3.44557852E-09 1.06183616E-11 5.51442883E+04 4.94977536E+01
 4
 CPD*CPD C 10 H 8 G 3E+02 2E+03 1E+03
 1
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 12 2

4.46869722E+04 5.78372545E+01-7.44864713E+00 1.01284503E-01-7.01210468E-
 05 3
 8.72805338E-09 7.29667500E-12 4.46869722E+04 5.78372545E+01
 4
 CPD*cyCC*CCCJ C 10 H 9 G 3E+02 2E+03 1E+03
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 12 2
 4.40666531E+04 6.08806525E+01-7.64852570E+00 1.04890622E-01-6.99375396E-
 05 3
 5.71592004E-09 8.86283367E-12 4.40666531E+04 6.08806525E+01
 4
 CPD*cyCC*CCJC C 10 H 9 G 3E+02 2E+03 1E+03
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 05 3
 -1.45047719E-09 1.14711853E-11 4.20111481E+04 5.99246855E+01
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 tricyclicC10H9 C 10 H 9 G 3E+02 2E+03 1E+03
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 Spiro45_C10H9 C 10 H 9 G 3E+02 2E+03 1E+03
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 11 2
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 CPDC*CC*CCJ C 10 H 11 G 3E+02 2E+03 1E+03
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 11 2
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 4.29602961E+04 5.01569908E+01-4.61889592E+00 9.46009076E-02-4.17862126E-
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 11 2
 2.96161353E+04 5.54462124E+01-6.40069364E+00 9.70366651E-02-3.97622659E-
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 11 2
 2.91487666E+04 5.27314253E+01-5.68768268E+00 9.42244077E-02-3.63530413E-
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 Indene3AH C 9 H 8 G 3E+02 2E+03 1E+03
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 11 2
 3.56053501E+04 5.77768727E+01-7.21087617E+00 8.99735161E-02-5.22882247E-
 05 3
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 C7H7 Benzyl rad T08/90C 7H 7 0 0G 200.000 6000.000 1000.
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 13 2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
 04 3
 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
 0.25317186E+05 4
 C*C(CJ)CC*C C 6 H 9 G 3E+02 2E+03 1E+03
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9.44029281E-01 5.60637118E-02-3.01901070E-05-1.26783371E-09 5.36277036E-
 12 2
 2.43043079E+04 2.08507646E+01 9.44029281E-01 5.60637118E-02-3.01901070E-
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 -1.26783371E-09 5.36277036E-12 2.43043079E+04 2.08507646E+01
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 13 2
 4.07373201E+03-3.00756024E+01 4.52393792E-01 3.63456797E-02 7.04032779E-
 05 3
 -1.28418017E-07 5.67812327E-11 7.56391136E+03 2.68770932E+01
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 13 2
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 13 2
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 C#CCcyCC*CC*C C 8 H 8 G 3E+02 2E+03 1E+03
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 C#CCCC*C 12/26/14 THERMC 6H 8 0 0G 300.000 5000.000
 1382.000 31
 1.60500327E+01 1.95004720E-02-6.82735194E-06 1.07658035E-09-6.31385498E-
 14 2
 2.22227970E+04-5.80128999E+01 4.08807006E-01 5.58885174E-02-4.07758983E-
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 C*C*CCC*C C6H8 C 6H 8O 0 G 300.000 5000.000
 1395.000 1
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 C*C*CCCJC*C C 7 H 9 G 3E+02 2E+03 1E+03
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 C*cy(CC*CC*CC) C 7 H 8 G 3E+02 2E+03 1E+03
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 C*C*CcyCC*CC*C C 8 H 8 G100.000 5000.000 959.19
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 13 2
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 05 3

-1.36921610E-07 6.94845065E-11 3.48586680E+04 3.48821049E+01
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 C*CCyCC*CC*CCJ C 8 H 9 G100.000 5000.000 1028.11
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 11 2
 2.82515807E+03 3.01659734E+01-6.21978642E-01 4.87010547E-02 4.39427575E-
 05 3
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 4

Ccy(CJCCCC) C 7 H 13 G 3E+02 2E+03 1E+03
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 1.89951139E+03 2.88156194E+01-4.73025824E-02 4.29587496E-02 5.69442582E-05 3
 -1.00732666E-07 4.20055410E-11 1.89951139E+03 2.88156194E+01
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 Ccy(CCCJCCC) C 7 H 13 G 3E+02 2E+03 1E+03
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 2.74748526E+03 2.90884542E+01-3.64028600E-01 4.70645814E-02 4.80143022E-05 3
 -9.34128015E-08 3.99070297E-11 2.74748526E+03 2.90884542E+01
 4
 Ccy(CCJCCCC) C 7 H 13 G 3E+02 2E+03 1E+03
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 2.93314409E+03 3.10879397E+01-8.17932107E-01 5.00039569E-02 4.07914326E-05 3
 -8.58074267E-08 3.70289703E-11 2.93314409E+03 3.10879397E+01
 4
 CJcy(CCCCC) C 7 H 13 G 3E+02 2E+03 1E+03
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 4.27502430E+03 3.35485112E+01-1.37323424E+00 5.40559305E-02 3.29257009E-05 3
 -7.96188634E-08 3.52699110E-11 4.27502430E+03 3.35485112E+01
 4
 C*CCC(C)CJC C 7 H 13 G 3E+02 2E+03 1E+03
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 1.19905412E+04 1.66769985E+01 3.16880912E+00 5.15666001E-02 9.11275666E-06 3
 -4.47830155E-08 2.09821836E-11 1.19905412E+04 1.66769985E+01
 4
 C*CCC(C)CCJ C 7 H 13 G 3E+02 2E+03 1E+03
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 1.35111492E+04 2.01289548E+01 2.16152886E+00 6.05156263E-02-7.97893486E-06 3
 -3.15351296E-08 1.72210371E-11 1.35111492E+04 2.01289548E+01
 4
 CCJCC(C)C*C C 7 H 13 G 3E+02 2E+03 1E+03
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 1.17709345E+04 4.80024866E+00 5.64108493E+00 3.97449941E-02 3.39267778E-05 3
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 C*CCCCJCC C 7 H 13 G 3E+02 2E+03 1E+03
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6.87131831E+00 2.81810065E-02 5.99653654E-05-9.26073607E-08 3.74567577E-
 11 2
 1.29226002E+04 3.77704736E+00 6.87131831E+00 2.81810065E-02 5.99653654E-
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 CJCCCC*CC C 7 H 13 G 3E+02 2E+03 1E+03
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 6.11286900E+00 3.59117596E-02 4.13285191E-05-7.41894847E-08 3.09102203E-
 11 2
 1.28763847E+04 3.75193029E+00 6.11286900E+00 3.59117596E-02 4.13285191E-
 05 3
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 CC*CCCCJC C 7 H 13 G 3E+02 2E+03 1E+03
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 7.12014926E+00 2.69627334E-02 5.84202106E-05-8.74373706E-08 3.46713668E-
 11 2
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 05 3
 -8.74373706E-08 3.46713668E-11 1.13557768E+04 2.99974017E-01
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 7.02705852E+00 2.92687355E-02 5.41257175E-05-8.44314583E-08 3.39286602E-
 11 2
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 05 3
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 C*CC(C)CCCJ C 7 H 13 G 3E+02 2E+03 1E+03
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 4.63380468E+00 4.86940203E-02 1.68350863E-05-5.51923691E-08 2.55279112E-
 11 2
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 05 3
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 0.14043980E+02 0.23493873E-01-0.85375367E-05 0.13890841E-08-0.83614420E-
 13 2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
 04 3
 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
 0.25317186E+05 4
 C7H7_4 C 7H 7 0 0G 200.000 6000.000 1000.
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 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
 04 3
 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
 0.25317186E+05 4
 cC7H7 C 7H 7 0 0G 200.000 6000.000 1000.
 1
 0.14043980E+02 0.23493873E-01-0.85375367E-05 0.13890841E-08-0.83614420E-
 13 2

0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
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 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
 0.25317186E+05 4
 C7H7_6 C 7H 7 0 0G 200.000 6000.000 1000.
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 13 2
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 04 3
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 0.25317186E+05 4
 C7H7_7 C 7H 7 0 0G 200.000 6000.000 1000.
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 13 2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
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 0.25317186E+05 4
 C7H7_8 C 7H 7 0 0G 200.000 6000.000 1000.
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 13 2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-
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 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
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 04 3
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 C#Ccy(C*CC*CC) C 7H 6 0 0G 300.000 5000.000 1000.
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 12 2
 0.33537602E+05-0.51359589E+02-0.54668241E+01 0.84791228E-01-0.69205664E-
 04 3
 0.17854783E-07 0.14455038E-11 0.37714207E+05 0.44820885E+02
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 04 3

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 -0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
 0.25317186E+05 4
 fulvenallene C 7H 6 0 0G 300.000 5000.000 1000.
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 0.17854783E-07 0.14455038E-11 0.37714207E+05 0.44820885E+02
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 C*CcyC*CC*CC C 7 H 8 G 3E+02 2E+03 1E+03
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 05 3
 -6.62030263E-08 3.35837139E-11 2.21168495E+04 2.86349787E+01
 4
 C*CcyC*CCC*C C 7 H 8 G 3E+02 2E+03 1E+03
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 2.39177229E+04 3.34899323E+01-1.95039399E+00 5.71919898E-02 1.24266425E-
 05 3
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 3.27225830E+04 4
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 04 3
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 CJ*C(C)CC*C C 6 H 9 G 3E+02 2E+03 1E+03
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 05 3
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 C6H5C*CCC C 10 H 12 G 3E+02 2E+03 1E+03
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 05 3
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 05 3
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 C6H5CCJC C 9 H 11 G 3E+02 2E+03 1E+03
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 4
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 C6H5CJCC*C C 10 H 11 G 3E+02 2E+03 1E+03
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 C6H5CJC*C C 9 H 9 G 3E+02 2E+03 1E+03
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 05 3
 3.97400000E-08-7.15500000E-12 2.80800000E+04 5.69900000E+01
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 C6H5CC*CC C 10 H 12 G 3E+02 2E+03 1E+03
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 06 3
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 05 3
 2.89800000E-08-4.36300000E-12 1.44300000E+04 5.42200000E+01
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 3.20088064E+04 2.57415557E+01-4.37183135E+00 1.07991713E-01-6.32702694E-
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 C6H5CJC*C-cy C 9 H 9 G 3E+02 2E+03 1E+03
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 1.65749493E-08 1.29659698E-12 3.96849528E+04 3.04766040E+01
 4
 C6H5CJC*CC-cy C 10 H 11 G 3E+02 2E+03 1E+03
 1
 -4.68041867E+00 1.09345633E-01-7.45949225E-05 1.49897627E-08 3.41062238E-
 12 2
 3.57618155E+04 2.88263310E+01-4.68041867E+00 1.09345633E-01-7.45949225E-
 05 3
 1.49897627E-08 3.41062238E-12 3.57618155E+04 2.88263310E+01
 4

M1H1Indene C 10 H 10 G 3E+02 2E+03 1E+03
1
-7.74983362E-01 4.26209008E-02 7.77230686E-06-4.07514457E-08 1.95478072E-
11 2
4.28253336E+03 3.30462342E+01-7.74983362E-01 4.26209008E-02 7.77230686E-
06 3
-4.07514457E-08 1.95478072E-11 4.28253336E+03 3.30462342E+01
4
C6H5CCCJ-cy C 9 H 11 G 3E+02 2E+03 1E+03
1
-1.63651664E+00 7.42021207E-02 1.33252645E-05-8.04177136E-08 4.06532736E-
11 2
2.78084981E+04 1.81213939E+01-1.63651664E+00 7.42021207E-02 1.33252645E-
05 3
-8.04177136E-08 4.06532736E-11 2.78084981E+04 1.81213939E+01
4
C6H5CCCCJ-cy C 10 H 13 G 3E+02 2E+03 1E+03
1
-2.92478011E+00 9.98147263E-02-3.58000183E-05-1.94616352E-08 1.27857629E-
11 2
1.65124139E+04 2.00450658E+01-2.92478011E+00 9.98147263E-02-3.58000183E-
05 3
-1.94616352E-08 1.27857629E-11 1.65124139E+04 2.00450658E+01
4
C6H5CCCCJC-cy C 10 H 13 G 3E+02 2E+03 1E+03
1
-3.85901333E+00 9.85357464E-02-1.83267248E-05-5.83456608E-08 3.44604249E-
11 2
2.41049675E+04 2.72492585E+01-3.85901333E+00 9.85357464E-02-1.83267248E-
05 3
-5.83456608E-08 3.44604249E-11 2.41049675E+04 2.72492585E+01
4
CPDcy (CCJC*CC) C 10 H 11 G250.000 5000.000 995.00
1
2.32414507E+01 3.18229957E-02-1.07493695E-05 1.66203512E-09-9.65438997E-
14 2
3.04381856E+04-1.00956740E+02 2.41914259E+00 2.50754487E-02 1.35775888E-
04 3
-1.87863332E-07 7.04734316E-11 3.90598613E+04 2.18962152E+01
4
CPD1cy (CCJC*CC) C 10 H 11 G250.000 5000.000 995.00
1
2.28623499E+01 3.24263112E-02-1.10580976E-05 1.72219186E-09-1.00589784E-
13 2
2.93880614E+04-9.81446763E+01 2.49999891E+00 2.70202867E-02 1.28635234E-
04 3
-1.80003482E-07 6.77001381E-11 3.77602535E+04 2.16978624E+01
4
CPD1C*CC*CCJ C 10 H 11 G250.000 5000.000 995.00
1
2.26679790E+01 3.29075899E-02-1.13730929E-05 1.78806572E-09-1.05193265E-
13 2
2.72846985E+04-9.52558756E+01 2.59339668E+00 4.00478554E-02 8.87499962E-
05 3
-1.39586047E-07 5.40801563E-11 3.49212433E+04 1.97909829E+01
4
C*CCJ*CCC*C C 7 H 9 G100.000 5000.000 813.02
1

1.08663456E+01 3.35903121E-02-1.28184031E-05 2.04624456E-09-1.24299300E-
 13 2
 3.84653163E+04-2.49889603E+01 1.25272797E+00 5.29138841E-02 3.14234951E-
 06 3
 -5.33624480E-08 2.99270589E-11 4.09531035E+04 2.50872005E+01
 4
 C*CCCJCC*C C 7 H 11 G 3E+02 2E+03 1E+03
 1
 5.04798317E+00 3.26612504E-02 4.07045905E-05-7.20803376E-08 2.99818570E-
 11 2
 2.84339968E+04 1.09955115E+01 5.04798317E+00 3.26612504E-02 4.07045905E-
 05 3
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 4
 C*CC*CCCJC C 7 H 11 G 3E+02 2E+03 1E+03
 1
 2.92892337E+00 4.07425309E-02 4.05818595E-05-8.43317551E-08 3.71624735E-
 11 2
 2.56735988E+04 1.85145607E+01 2.92892337E+00 4.07425309E-02 4.05818595E-
 05 3
 -8.43317551E-08 3.71624735E-11 2.56735988E+04 1.85145607E+01
 4
 CC*CC*CCCJ C 7 H 11 G 3E+02 2E+03 1E+03
 1
 3.95930634E+00 4.09723898E-02 3.48326142E-05-7.66167898E-08 3.40723875E-
 11 2
 2.54654587E+04 1.10435794E+01 3.95930634E+00 4.09723898E-02 3.48326142E-
 05 3
 -7.66167898E-08 3.40723875E-11 2.54654587E+04 1.10435794E+01
 4
 C*CC*CC*CC C 7 H 10 G 3E+02 2E+03 1E+03
 1
 -3.13573025E-01 5.54840972E-02 2.03845518E-05-7.67282618E-08 3.74550956E-
 11 2
 1.45300471E+04 2.94093713E+01-3.13573025E-01 5.54840972E-02 2.03845518E-
 05 3
 -7.67282618E-08 3.74550956E-11 1.45300471E+04 2.94093713E+01
 4
 C*CC*CCC*C C 7 H 10 G 3E+02 2E+03 1E+03
 1
 2.53402070E+00 4.49680793E-02 2.47539275E-05-6.84457650E-08 3.17234244E-
 11 2
 1.73676225E+04 1.83584856E+01 2.53402070E+00 4.49680793E-02 2.47539275E-
 05 3
 -6.84457650E-08 3.17234244E-11 1.73676225E+04 1.83584856E+01
 4
 JOOcy(CC*CCC) C 5 O 2 H 7 G 3E+02 2E+03 1E+03
 1
 -4.25155128E+00 9.13446161E-02-1.30831640E-04 1.13786250E-07-4.08813202E-
 11 2
 1.01406562E+04 4.41505592E+01-4.25155128E+00 9.13446161E-02-1.30831640E-
 04 3
 1.13786250E-07-4.08813202E-11 1.01406562E+04 4.41505592E+01
 4
 JOcy(CC*CCC) C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 -2.60598171E-02 4.80359624E-02-3.06021603E-05 1.56168144E-08-5.75583617E-
 12 2

9.56544838E+03 2.59946430E+01-2.60598171E-02 4.80359624E-02-3.06021603E-
 05 3
 1.56168144E-08-5.75583617E-12 9.56544838E+03 2.59946430E+01
 4
 HOOcy(CC*CCC) C 5 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 -4.21572069E+00 9.27414776E-02-1.20091913E-04 9.72763990E-08-3.40428276E-
 11 2
 -8.16365160E+03 4.30747450E+01-4.21572069E+00 9.27414776E-02-1.20091913E-
 04 3
 9.72763990E-08-3.40428276E-11-8.16365160E+03 4.30747450E+01
 4
 O*cy(CC*CCC) C 5 O 1 H 6 G 3E+02 2E+03 1E+03
 1
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 11 2
 -1.23754651E+04 3.82105557E+01-3.11403646E+00 7.19485244E-02-9.76194313E-
 05 3
 8.69345593E-08-3.22536178E-11-1.23754651E+04 3.82105557E+01
 4
 O*cy(CC*CCC*C) C 6 O 1 H 6 G 3E+02 2E+03 1E+03
 1
 -3.57525957E+00 1.18128310E-01-2.06330708E-04 1.89169155E-07-6.65436791E-
 11 2
 -6.78694671E+03 2.02709628E+01-3.57525957E+00 1.18128310E-01-2.06330708E-
 04 3
 1.89169155E-07-6.65436791E-11-6.78694671E+03 2.02709628E+01
 4
 O*cy(CC*CC*CC) C 6 O 1 H 6 G 3E+02 2E+03 1E+03
 1
 -3.55610409E+00 9.59386879E-02-1.23521640E-04 8.70793159E-08-2.53997314E-
 11 2
 -4.00821706E+03 2.28588727E+01-3.55610409E+00 9.59386879E-02-1.23521640E-
 04 3
 8.70793159E-08-2.53997314E-11-4.00821706E+03 2.28588727E+01
 4
 HOOcy(CC*CCC*C) C 6 H 8 O 2 G100.000 5000.000 2170.58
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 -4.12051947E+01 9.36389088E-02-2.93169400E-05 8.75443910E-10 1.17414157E-
 13 2
 2.79096698E+04 2.86143076E+02-9.64040220E-01 6.92756266E-02-4.68911027E-
 05 3
 1.68419074E-08-2.93882180E-12-1.28973378E+03 3.37955268E+01
 4
 HOOcy(CC*CC*CC) C 6 H 8 O 2 G100.000 5000.000 925.40
 1
 1.36624484E+01 3.28361035E-02-1.42206754E-05 2.79948853E-09-2.05192496E-
 13 2
 -5.57031630E+03-4.57761175E+01-1.70216217E+00 6.10734619E-02 1.88765694E-
 06 3
 -5.33827791E-08 2.70153415E-11-1.09201130E+03 3.59899798E+01
 4
 JOcy(CC*CC*CC) C 6 H 7 O 1 G100.000 5000.000 870.15
 1
 1.03026454E+01 3.07901026E-02-1.35495219E-05 2.70830161E-09-2.00950323E-
 13 2
 1.37243400E+04-2.99720075E+01-1.03603278E-01 3.32948157E-02 6.02769036E-
 05 3

-1.13723595E-07 5.04515216E-11 1.72515319E+04 2.86461524E+01
 4
 JOcy(CC*CCC*C) C 6 H 7 O 1 G100.000 5000.000 930.59
 1
 1.05024700E+01 3.06560923E-02-1.34773493E-05 2.67939854E-09-1.97536527E-
 13 2
 1.36109854E+04-2.84944750E+01 1.39626710E+00 2.82344054E-02 5.74209108E-
 05 3
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 4
 HOcy(CCJCC*CC) C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
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 13 2
 1.76997612E+03 4.19565329E+01-3.24696327E+00 7.32217880E-02-4.82998696E-
 05 3
 1.13796902E-08 6.65928138E-13 1.76997612E+03 4.19565329E+01
 4
 HOcyCCJCC*C C 5 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 -3.73681616E+00 7.10926491E-02-7.30507926E-05 4.59577903E-08-1.32707214E-
 11 2
 6.83857456E+03 4.30989747E+01-3.73681616E+00 7.10926491E-02-7.30507926E-
 05 3
 4.59577903E-08-1.32707214E-11 6.83857456E+03 4.30989747E+01
 4
 O*CCC*CCC*O C 6 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 3.96182618E+00 4.63682936E-02-7.34276694E-06-2.05555091E-08 1.09895539E-
 11 2
 -2.79563062E+04 1.59748873E+01 3.96182618E+00 4.63682936E-02-7.34276694E-
 06 3
 -2.05555091E-08 1.09895539E-11-2.79563062E+04 1.59748873E+01
 4
 O*CCPCCCCJ C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 4.42534830E-01 9.50552724E-02-9.82205634E-05 6.30857379E-08-1.86442701E-
 11 2
 -1.93530409E+04 3.29170580E+01 4.42534830E-01 9.50552724E-02-9.82205634E-
 05 3
 6.30857379E-08-1.86442701E-11-1.93530409E+04 3.29170580E+01
 4
 O*CCPC*CCCJ C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 8.16682257E+00 5.34344317E-02-3.59584427E-05 1.74690635E-08-5.62980839E-
 12 2
 -3.59841891E+03-3.36103709E+00 8.16682257E+00 5.34344317E-02-3.59584427E-
 05 3
 1.74690635E-08-5.62980839E-12-3.59841891E+03-3.36103709E+00
 4
 O*CCCC*O C 5 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 1.03376956E+01 3.37780009E-03 7.34474615E-05-8.95093688E-08 3.31206845E-
 11 2
 -4.10452907E+04-1.36454771E+01 1.03376956E+01 3.37780009E-03 7.34474615E-
 05 3
 -8.95093688E-08 3.31206845E-11-4.10452907E+04-1.36454771E+01
 4

O*CCCCJOOH C 5 O 3 H 9 G 3E+02 2E+03 1E+03
1
6.45890582E+00 5.64988432E-02-4.34654987E-05 2.32518854E-08-7.23807490E-
12 2
-1.89099751E+04 3.79631948E+00 6.45890582E+00 5.64988432E-02-4.34654987E-
05 3
2.32518854E-08-7.23807490E-12-1.89099751E+04 3.79631948E+00
4
HOcyCCJC*CC C 5 O 1 H 7 G 3E+02 2E+03 1E+03
1
-4.42152571E+00 8.22122075E-02-9.41892326E-05 6.40626942E-08-1.91925445E-
11 2
-3.09974239E+03 4.04235841E+01-4.42152571E+00 8.22122075E-02-9.41892326E-
05 3
6.40626942E-08-1.91925445E-11-3.09974239E+03 4.04235841E+01
4
JOcy(CCPC*CC) C 5 O 3 H 7 G 3E+02 2E+03 1E+03
1
-5.74288375E+00 1.10228255E-01-1.55286183E-04 1.26669887E-07-4.31925282E-
11 2
-1.03712260E+03 5.10823610E+01-5.74288375E+00 1.10228255E-01-1.55286183E-
04 3
1.26669887E-07-4.31925282E-11-1.03712260E+03 5.10823610E+01
4
O*CC*CCCCJOOH C 6 O 3 H 9 G 3E+02 2E+03 1E+03
1
-3.03060097E+00 1.34482315E-01-2.13327893E-04 1.85483068E-07-6.40120923E-
11 2
-9.17234602E+03 4.22585438E+01-3.03060097E+00 1.34482315E-01-2.13327893E-
04 3
1.85483068E-07-6.40120923E-11-9.17234602E+03 4.22585438E+01
4
O*CC*CCCC*O C 6 O 2 H 8 G 3E+02 2E+03 1E+03
1
8.48188849E-01 8.13612717E-02-9.64149329E-05 7.27218141E-08-2.36533329E-
11 2
-3.13076616E+04 2.55098945E+01 8.48188849E-01 8.13612717E-02-9.64149329E-
05 3
7.27218141E-08-2.36533329E-11-3.13076616E+04 2.55098945E+01
4
JOcy(CCPCCC) C 5 O 3 H 9 G 3E+02 2E+03 1E+03
1
2.14070676E-01 6.64822155E-02-3.10747514E-05-7.71766650E-09 8.19320555E-
12 2
-1.57040186E+04 2.90252812E+01 2.14070676E-01 6.64822155E-02-3.10747514E-
05 3
-7.71766650E-09 8.19320555E-12-1.57040186E+04 2.90252812E+01
4
O*CC*CCCJOOH C 5 O 3 H 7 G 3E+02 2E+03 1E+03
1
-4.66635369E+00 1.32446554E-01-2.26688864E-04 2.03059458E-07-7.07657202E-
11 2
-6.04253780E+03 4.78381021E+01-4.66635369E+00 1.32446554E-01-2.26688864E-
04 3
2.03059458E-07-7.07657202E-11-6.04253780E+03 4.78381021E+01
4
HOcyCCJCCC C 5 O 1 H 9 G 3E+02 2E+03 1E+03
1

2.22013827E+00 2.73466096E-02 5.11606394E-05-8.84297636E-08 3.81150123E-
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 4
 JOcyCCPCCC*C C 6 O 3 H 9 G 3E+02 2E+03 1E+03
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 -3.21823337E+00 1.09858786E-01-1.37622508E-04 1.07459678E-07-3.68095213E-
 11 2
 -7.19079455E+03 3.92343725E+01-3.21823337E+00 1.09858786E-01-1.37622508E-
 04 3
 1.07459678E-07-3.68095213E-11-7.19079455E+03 3.92343725E+01
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 HOcy(CCJC*CCC) C 6 O 1 H 9 G 3E+02 2E+03 1E+03
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 11 2
 -8.34399902E+03 4.19230878E+01-5.35289461E+00 1.03901173E-01-1.15741261E-
 04 3
 7.30738448E-08-2.00205729E-11-8.34399902E+03 4.19230878E+01
 4
 JOOcyCCOHCCC C 5 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 7.91147251E-01 6.35535382E-02-3.40236478E-05-3.05034794E-10 4.92700742E-
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 -2.51813118E+04 2.76109152E+01 7.91147251E-01 6.35535382E-02-3.40236478E-
 05 3
 -3.05034794E-10 4.92700742E-12-2.51813118E+04 2.76109152E+01
 4
 JOOcyCCOHCCCC C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
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 11 2
 -3.12455544E+04 2.95345871E+01-4.97116216E-01 8.91661437E-02-8.31489307E-
 05 3
 6.06510437E-08-2.29405032E-11-3.12455544E+04 2.95345871E+01
 4
 JOOcyCCOHC*CCC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
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 11 2
 -1.57586724E+04 5.11674987E+01-6.09717607E+00 1.28988543E-01-1.79787109E-
 04 3
 1.43093670E-07-4.72867546E-11-1.57586724E+04 5.11674987E+01
 4
 JOOcyCCOHC*CC C 5 O 3 H 7 G 3E+02 2E+03 1E+03
 1
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 11 2
 -1.05144157E+04 4.96679950E+01-5.16580718E+00 1.07299578E-01-1.58235080E-
 04 3
 1.34082519E-07-4.64587263E-11-1.05144157E+04 4.96679950E+01
 4
 O*CCPCCJC*C C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 -3.71181872E+00 1.10324649E-01-1.36124570E-04 9.83269475E-08-3.04966702E-
 11 2

-1.15227403E+04 5.02251606E+01-3.71181872E+00 1.10324649E-01-1.36124570E-
04 3
9.83269475E-08-3.04966702E-11-1.15227403E+04 5.02251606E+01
4
JOcy(CCPCC*CC) C 6 O 3 H 9 G 3E+02 2E+03 1E+03
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-5.25303086E+00 1.12357394E-01-1.30535260E-04 9.20917873E-08-2.92558786E-
11 2
-6.10572104E+03 4.99399191E+01-5.25303086E+00 1.12357394E-01-1.30535260E-
04 3
9.20917873E-08-2.92558786E-11-6.10572104E+03 4.99399191E+01
4
JOOcyCC*CCOHCC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
1
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11 2
-1.59343306E+04 5.38094443E+01-7.51839785E+00 1.48548370E-01-2.26090060E-
04 3
1.86682920E-07-6.20514326E-11-1.59343306E+04 5.38094443E+01
4
HOcyCCJCCC*C C 6 O 1 H 9 G 3E+02 2E+03 1E+03
1
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11 2
1.59431793E+03 4.45984785E+01-4.66818505E+00 9.27816145E-02-9.46028213E-
05 3
5.49689409E-08-1.40987498E-11 1.59431793E+03 4.45984785E+01
4
O*CCCCC*O C 6 O 2 H 10 G 3E+02 2E+03 1E+03
1
1.19734484E+01 5.41356120E-03 8.68084328E-05-1.07085759E-07 3.98743124E-
11 2
-4.41750989E+04-1.92250353E+01 1.19734484E+01 5.41356120E-03 8.68084328E-
05 3
-1.07085759E-07 3.98743124E-11-4.41750989E+04-1.92250353E+01
4
JOOcyCCOHCCC*C C 6 O 3 H 9 G 3E+02 2E+03 1E+03
1
-6.09717607E+00 1.28988543E-01-1.79787109E-04 1.43093670E-07-4.72867546E-
11 2
-1.57586724E+04 5.11674987E+01-6.09717607E+00 1.28988543E-01-1.79787109E-
04 3
1.43093670E-07-4.72867546E-11-1.57586724E+04 5.11674987E+01
4
JOcyCCPCCCC C 6 O 3 H 11 G 3E+02 2E+03 1E+03
1
-1.07419279E+00 9.20948210E-02-8.02000343E-05 5.32384120E-08-1.96743051E-
11 2
-2.17682613E+04 3.09489531E+01-1.07419279E+00 9.20948210E-02-8.02000343E-
05 3
5.32384120E-08-1.96743051E-11-2.17682613E+04 3.09489531E+01
4
JOOcyCCOHCC*C C 5 O 3 H 7 G 3E+02 2E+03 1E+03
1
-5.16580718E+00 1.07299578E-01-1.58235080E-04 1.34082519E-07-4.64587263E-
11 2
-1.05144157E+04 4.96679950E+01-5.16580718E+00 1.07299578E-01-1.58235080E-
04 3

1.34082519E-07-4.64587263E-11-1.05144157E+04 4.96679950E+01
 4
 JOcyCCPCC*C C 5 O 3 H 7 G 3E+02 2E+03 1E+03
 1
 -2.28686448E+00 8.81698205E-02-1.16070479E-04 9.84485277E-08-3.59814930E-11 2
 -1.94653792E+03 3.77348688E+01-2.28686448E+00 8.81698205E-02-1.16070479E-04 3
 9.84485277E-08-3.59814930E-11-1.94653792E+03 3.77348688E+01
 4
 JOOcyCCOHCC*CC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 -4.67595429E+00 1.09428717E-01-1.33484157E-04 9.95044190E-08-3.25220767E-11 2
 -1.55830142E+04 4.85255531E+01-4.67595429E+00 1.09428717E-01-1.33484157E-04 3
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 4
 O*CCPCJC*C C 5 O 3 H 7 G 3E+02 2E+03 1E+03
 1
 -5.44066218E+00 1.10594890E-01-1.53780034E-04 1.18909250E-07-3.79930048E-11 2
 -7.18444526E+03 5.63757083E+01-5.44066218E+00 1.10594890E-01-1.53780034E-04 3
 1.18909250E-07-3.79930048E-11-7.18444526E+03 5.63757083E+01
 4
 O*CCPCCCJ C 5 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 -1.19321788E+00 9.30195113E-02-1.11581535E-04 8.06621279E-08-2.53978980E-11 2
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 8.06621279E-08-2.53978980E-11-1.62232327E+04 3.84966162E+01
 4
 HOcy(CCJCCCC) C 6 O 1 H 11 G 3E+02 2E+03 1E+03
 1
 9.31874801E-01 5.29592152E-02 2.03535653E-06-2.74736851E-08 1.02475016E-11 2
 -1.38925641E+04 2.22724196E+01 9.31874801E-01 5.29592152E-02 2.03535653E-06 3
 -2.74736851E-08 1.02475016E-11-1.38925641E+04 2.22724196E+01
 4
 JOcyCCPC*CCC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 -6.67425264E+00 1.31917220E-01-1.76838212E-04 1.35681038E-07-4.40205565E-11 2
 -6.28137923E+03 5.25818647E+01-6.67425264E+00 1.31917220E-01-1.76838212E-04 3
 1.35681038E-07-4.40205565E-11-6.28137923E+03 5.25818647E+01
 4
 O*CCCCCJOOH C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 8.09465854E+00 5.85346043E-02-3.01045273E-05 5.67549547E-09-4.84446962E-13 2
 -2.20397833E+04-1.78323879E+00 8.09465854E+00 5.85346043E-02-3.01045273E-05 3
 5.67549547E-09-4.84446962E-13-2.20397833E+04-1.78323879E+00
 4

O*CCCC*CCJOOH C 6 O 3 H 9 G 3E+02 2E+03 1E+03
1
3.34207317E+00 7.28764405E-02-5.83663095E-05 2.67572177E-08-6.18081124E-
12 2
-1.42677517E+04 1.89358020E+01 3.34207317E+00 7.28764405E-02-5.83663095E-
05 3
2.67572177E-08-6.18081124E-12-1.42677517E+04 1.89358020E+01
4
O*CCC*CCJOOH C 5 O 3 H 7 G 3E+02 2E+03 1E+03
1
-1.07634153E-01 8.34481822E-02-9.82981522E-05 6.81000330E-08-2.07479649E-
11 2
-1.05979475E+04 3.18183616E+01-1.07634153E-01 8.34481822E-02-9.82981522E-
05 3
6.81000330E-08-2.07479649E-11-1.05979475E+04 3.18183616E+01
4
JOOcyCC*CCOHC C 5 O 3 H 7 G 3E+02 2E+03 1E+03
1
-6.58702896E+00 1.26859404E-01-2.04538031E-04 1.77671770E-07-6.12234042E-
11 2
-1.06900739E+04 5.23099405E+01-6.58702896E+00 1.26859404E-01-2.04538031E-
04 3
1.77671770E-07-6.12234042E-11-1.06900739E+04 5.23099405E+01
4
O*CCC*CCCJOOH C 6 O 3 H 9 G 3E+02 2E+03 1E+03
1
1.89699097E+00 8.68818339E-02-9.76848558E-05 6.84393198E-08-2.15556798E-
11 2
-6.36098668E+03 2.61136825E+01 1.89699097E+00 8.68818339E-02-9.76848558E-
05 3
6.84393198E-08-2.15556798E-11-6.36098668E+03 2.61136825E+01
4
C6H5CH2OOH OC 7H 8O 2 G 0300.00 5000.00 1000.00
1
0.11269509E+02 0.37149373E-01-0.14254149E-04 0.24727249E-08-0.16134546E-
12 2
-0.92585859E+04-0.28077469E+02-0.40976644E+01 0.81227809E-01-0.52230549E-
04 3
0.90553014E-08 0.24712715E-11-0.54439961E+04 0.50132618E+02
4
C6H5CH2O OC 7H 7O 1 G 0300.00 5000.00 1000.00
1
0.10762488E+02 0.30655593E-01-0.10738148E-04 0.17451247E-08-0.10868436E-
12 2
0.80504043E+04-0.30423080E+02-0.68475990E+01 0.81168644E-01-0.59274342E-
04 3
0.18262895E-07-0.10218114E-11 0.12635879E+05 0.59700500E+02
4
C6H5CHO OC 7H 6O 1 G 0300.00 5000.00 1000.00
1
0.27822605E+02 0.62637692E-02-0.14661670E-05 0.18006827E-09-0.93566283E-
14 2
-0.15845393E+05-0.12738686E+03-0.34431257E+01 0.66832952E-01-0.34990375E-
04 3
0.32432945E-08 0.11444751E-11-0.46860913E+04 0.43472546E+02
4
C6H5C2H2 OC 8H 7O 0 G 0300.00 5000.00 1000.00
1

0.14594848E+02 0.23882853E-01-0.75691555E-05 0.11463872E-08-0.68014537E-
 13 2
 0.34474055E+05-0.52785233E+02-0.18172119E+01 0.60460128E-01-0.27423970E-
 04 3
 -0.40506389E-08 0.48146214E-11 0.39538484E+05 0.34447075E+02
 4
 C6H5CO OC 7H 50 1 G 0300.00 5000.00 1000.00
 1
 0.26774740E+02 0.46817856E-02-0.78398284E-06 0.73234342E-10-0.30958701E-
 14 2
 0.56113867E+03-0.12106253E+03-0.22810972E+01 0.54210059E-01-0.15234797E-
 04 3
 -0.10887473E-07 0.49300798E-11 0.11423319E+05 0.39765499E+02
 4
 C6H5CPC C 8H 100 2 G 0300.00 5000.00
 1000.00 1
 -0.31565318E+01 0.72488472E-01-0.31781656E-04 0.60659939E-08-0.42418182E-
 12 2
 -0.75729609E+04 0.52722046E+02-0.80470219E+01 0.11141342E+00-0.84831234E-
 04 3
 0.23181402E-07 0.13341983E-11-0.90922773E+04 0.67959465E+02
 4
 C6H5C(OJ)C C 8H 90 1 G 0300.00 5000.00
 1000.00 1
 -0.26841152E+01 0.63683085E-01-0.26554239E-04 0.48910964E-08-0.33337355E-
 12 2
 0.11209342E+05 0.45193958E+02-0.10515040E+02 0.10946906E+00-0.87473454E-
 04 3
 0.28099876E-07-0.67344112E-12 0.10719505E+05 0.76310471E+02
 4
 C*CC*CCJC*O C 6 O 1 H 7 G 3E+02 2E+03 1E+03
 1
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 11 2
 6.16178333E+03 5.38645186E+01-6.65969890E+00 1.02840371E-01-1.21564268E-
 04 3
 7.87877840E-08-2.12975659E-11 6.16178333E+03 5.38645186E+01
 4
 CJCCCC*O C 5 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 7.35545113E+00 1.75821480E-02 4.60481335E-05-6.73046845E-08 2.65977459E-
 11 2
 -5.65564031E+03-1.84089612E+00 7.35545113E+00 1.75821480E-02 4.60481335E-
 05 3
 -6.73046845E-08 2.65977459E-11-5.65564031E+03-1.84089612E+00
 4
 CCJCCC*O C 5 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 4.44225442E+00 2.61950045E-02 1.81981891E-05-3.94081422E-08 1.68644862E-
 11 2
 8.66778836E+03 1.41764447E+01 4.44225442E+00 2.61950045E-02 1.81981891E-
 05 3
 -3.94081422E-08 1.68644862E-11 8.66778836E+03 1.41764447E+01
 4
 C*CCJCCy(COC) C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 1.14335524E+01-1.28369225E-02 1.38383700E-04-1.66683717E-07 6.32167061E-
 11 2

8.50153520E+03-2.14091600E+01 1.14335524E+01-1.28369225E-02 1.38383700E-
 04 3
 -1.66683717E-07 6.32167061E-11 8.50153520E+03-2.14091600E+01
 4
 C*CCJC (OH)CC*O C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 3.57152932E+00 6.88360651E-02-5.05017149E-05 1.43894802E-08 5.39479280E-
 13 2
 -2.60071927E+04 1.10496775E+01 3.57152932E+00 6.88360651E-02-5.05017149E-
 05 3
 1.43894802E-08 5.39479280E-13-2.60071927E+04 1.10496775E+01
 4
 CJCCcy (COC) C 6 O 1 H 11 G 3E+02 2E+03 1E+03
 1
 1.32518231E+01-1.33412819E-02 1.46662805E-04-1.76325307E-07 6.68554684E-
 11 2
 2.71856520E+03-2.90826362E+01 1.32518231E+01-1.33412819E-02 1.46662805E-
 04 3
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 4
 CJCC*CCC*O C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 5.23258422E+00 3.65496084E-02 1.21412226E-05-3.82392623E-08 1.70914494E-
 11 2
 6.39142951E+03 8.84679708E+00 5.23258422E+00 3.65496084E-02 1.21412226E-
 05 3
 -3.82392623E-08 1.70914494E-11 6.39142951E+03 8.84679708E+00
 4
 CC*CCJCC*O C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 7.17293319E+00 2.01222685E-02 5.11300001E-05-7.52394848E-08 2.97126115E-
 11 2
 -3.00247854E+03-8.45590537E-01 7.17293319E+00 2.01222685E-02 5.11300001E-
 05 3
 -7.52394848E-08 2.97126115E-11-3.00247854E+03-8.45590537E-01
 4
 C*CCCJCC*O C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 6.49862582E+00 2.45077208E-02 4.00486232E-05-6.45950315E-08 2.60606798E-
 11 2
 5.97034116E+03 6.13667620E+00 6.49862582E+00 2.45077208E-02 4.00486232E-
 05 3
 -6.45950315E-08 2.60606798E-11 5.97034116E+03 6.13667620E+00
 4
 CJC (OH)CCC*O C 5 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 7.40816100E+00 3.09374669E-02 2.09100092E-05-4.76358056E-08 2.09958777E-
 11 2
 -2.61293285E+04-1.77928149E+00 7.40816100E+00 3.09374669E-02 2.09100092E-
 05 3
 -4.76358056E-08 2.09958777E-11-2.61293285E+04-1.77928149E+00
 4
 HOCCJCCcy (COC) C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 1.42914002E+01-8.87811966E-03 1.37071909E-04-1.66566832E-07 6.32405044E-
 11 2
 -1.77657046E+04-2.95949512E+01 1.42914002E+01-8.87811966E-03 1.37071909E-
 04 3

-1.66566832E-07 6.32405044E-11-1.77657046E+04-2.95949512E+01
 4
 HOCCJCCC*O C 5 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 8.39502830E+00 2.20453102E-02 3.64572379E-05-5.75462095E-08 2.29827818E-
 11 2
 -2.61399101E+04-2.35321113E+00 8.39502830E+00 2.20453102E-02 3.64572379E-
 05 3
 -5.75462095E-08 2.29827818E-11-2.61399101E+04-2.35321113E+00
 4
 CCJCCcy (COC) C 6 O 1 H 11 G 3E+02 2E+03 1E+03
 1
 1.42591033E+01-2.22903082E-02 1.63754496E-04-1.89573193E-07 7.06166149E-
 11 2
 1.19795729E+03-3.25345924E+01 1.42591033E+01-2.22903082E-02 1.63754496E-
 04 3
 -1.89573193E-07 7.06166149E-11 1.19795729E+03-3.25345924E+01
 4
 C*CC (OH) CJCC*O C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 4.16314814E+00 6.00225088E-02-3.36577680E-05-7.09511352E-10 5.71859577E-
 12 2
 -1.48603890E+04 1.42960575E+01 4.16314814E+00 6.00225088E-02-3.36577680E-
 05 3
 -7.09511352E-10 5.71859577E-12-1.48603890E+04 1.42960575E+01
 4
 CJC (OH) C*CCC*O C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 1.42502437E+00 8.08802841E-02-7.96122996E-05 4.11408794E-08-8.08640512E-
 12 2
 -1.37559983E+04 2.31800272E+01 1.42502437E+00 8.08802841E-02-7.96122996E-
 05 3
 4.11408794E-08-8.08640512E-12-1.37559983E+04 2.31800272E+01
 4
 C*CCJCCC*O C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 7.17293319E+00 2.01222685E-02 5.11300001E-05-7.52394848E-08 2.97126115E-
 11 2
 -3.00247854E+03 2.53021752E-01 7.17293319E+00 2.01222685E-02 5.11300001E-
 05 3
 -7.52394848E-08 2.97126115E-11-3.00247854E+03 2.53021752E-01
 4
 HOCCJC*CCC*O C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 3.14840389E+00 6.35478594E-02-3.89005592E-05 5.74612866E-09 2.74335385E-
 12 2
 -2.35292387E+04 1.72887613E+01 3.14840389E+00 6.35478594E-02-3.89005592E-
 05 3
 5.74612866E-09 2.74335385E-12-2.35292387E+04 1.72887613E+01
 4
 CJC (OH) CCcy (COC) C 6 O 2 H 11 G 3E+02 2E+03 1E+03
 1
 1.33045330E+01 1.40369884E-05 1.21524680E-04-1.56656428E-07 6.12536003E-
 11 2
 -1.77551229E+04-2.90210215E+01 1.33045330E+01 1.40369884E-05 1.21524680E-
 04 3
 -1.56656428E-07 6.12536003E-11-1.77551229E+04-2.90210215E+01
 4

C*CC(OH)C*C C 5 O 1 H 8 G 3E+02 2E+03 1E+03
 1
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 11 2
 -9.44108837E+03 1.19285347E+01 3.63927619E+00 3.91380867E-02-9.56492856E-
 07 3
 -2.77640555E-08 1.45566944E-11-9.44108837E+03 1.19285347E+01
 4
 C4H71-4 070114H 7C 4 0 0g 300.000 2500.0001000.000
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 0.40415874E+01 0.28606180E-01-0.14108448E-04 0.34089804E-08-0.32725829E-
 12 2
 0.23388023E+05 0.69514360E+01 0.17970406E+01 0.29896524E-01-0.15524820E-
 05 3
 -0.17429736E-07 0.89120343E-11 0.24163896E+05 0.19524303E+02
 HHC 2 P 4
 C4H71-3 052114H 7C 4 0 0g 300.000 2500.0001000.000
 1
 0.35669293E+01 0.30164506E-01-0.15129679E-04 0.37195191E-08-0.36344620E-
 12 2
 0.14296935E+05 0.69067054E+01 0.13044622E+01 0.30223139E-01 0.14855871E-
 05 3
 -0.21546482E-07 0.10493627E-10 0.15136749E+05 0.19876741E+02
 HHC 1 P 4
 C*CCCOOJ C 4 H 7 O 2 G100.000 5000.000 1553.29
 1
 -1.94149058E+01 7.45644635E-02-3.49656824E-05 5.06126012E-09-2.55665738E-
 13 2
 1.58834992E+04 1.45731646E+02 1.14069142E+00 5.09071392E-02-4.03926016E-
 05 3
 1.95249914E-08-4.53662056E-12 5.96589349E+03 2.61416740E+01
 4
 JOOcy(CCCCC) C 5 H 9 O 2 G100.000 5000.000 789.47
 1
 7.51448545E+00 3.85532690E-02-1.57308891E-05 2.99087895E-09-2.15184329E-
 13 2
 -7.55282884E+03-9.59390296E+00-3.21000782E-01 3.67605242E-02 6.65114533E-
 05 3
 -1.33031192E-07 6.39399952E-11-5.02260157E+03 3.45448697E+01
 4
 cy(CC*CcyCOCC) C 6 H 8 O 1 G100.000 5000.000 2124.35
 1
 -4.57927271E+01 1.00291941E-01-3.31812663E-05 1.03561961E-09 1.33775893E-
 13 2
 1.52877081E+04 2.75965011E+02-9.18027098E-01 6.94531992E-02-4.92932349E-
 05 3
 1.79816862E-08-3.25971313E-12-1.58855869E+04-2.83768307E+00
 4
 HOOcy(CC*CC*C) C 5 H 6 O 2 G100.000 5000.000 900.86
 1
 1.24545606E+01 2.54702764E-02-1.13279674E-05 2.27085991E-09-1.68558430E-
 13 2
 -1.50819543E+03-3.89312433E+01 7.43913153E-03 4.38475871E-02 1.94982833E-
 05 3
 -6.59991937E-08 3.13924046E-11 2.23133307E+03 2.81276153E+01
 4
 C*CC*CC*CJ C 6 H 7 G 3E+02 2E+03 1E+03
 1

-2.15056514E+00 6.08067933E-02-1.90398195E-05-3.22643057E-08 2.11997813E-
 11 2
 4.89534834E+04 3.54131601E+01-2.15056514E+00 6.08067933E-02-1.90398195E-
 05 3
 -3.22643057E-08 2.11997813E-11 4.89534834E+04 3.54131601E+01
 4
 JOOCcy (CC*CCC) C 6 O 2 H 9 G 3E+02 2E+03 1E+03
 1
 -6.07690078E-01 7.63100781E-02-8.08792513E-05 6.37340995E-08-2.35792386E-
 11 2
 7.65958003E+03 3.19614110E+01-6.07690078E-01 7.63100781E-02-8.08792513E-
 05 3
 6.37340995E-08-2.35792386E-11 7.65958003E+03 3.19614110E+01
 4
 CJCCC*CC*O C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -2.13405566E+00 9.55656196E-02-1.23814261E-04 9.49264984E-08-3.01762715E-
 11 2
 4.08198875E+03 3.66213282E+01-2.13405566E+00 9.55656196E-02-1.23814261E-
 04 3
 9.49264984E-08-3.01762715E-11 4.08198875E+03 3.66213282E+01
 4
 JOcy (CC*CCCC) C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -9.57428710E-01 6.97249278E-02-5.21541890E-05 2.46279649E-08-6.58386454E-
 12 2
 4.32119175E+03 2.74941468E+01-9.57428710E-01 6.97249278E-02-5.21541890E-
 05 3
 2.46279649E-08-6.58386454E-12 4.32119175E+03 2.74941468E+01
 4
 HOOcy (CCC*CCC) C 6 O 2 H 10 G 3E+02 2E+03 1E+03
 1
 -3.72586780E+00 9.48706165E-02-9.53409897E-05 6.26982989E-08-2.01061780E-
 11 2
 -1.32322500E+04 4.19323031E+01-3.72586780E+00 9.48706165E-02-9.53409897E-
 05 3
 6.26982989E-08-2.01061780E-11-1.32322500E+04 4.19323031E+01
 4
 JOcy (CCC*CCC) C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -2.99222620E+00 7.22235358E-02-4.50669415E-05 9.26007399E-09 9.69778202E-
 13 2
 5.40626526E+03 3.81996934E+01-2.99222620E+00 7.22235358E-02-4.50669415E-
 05 3
 9.26007399E-09 9.69778202E-13 5.40626526E+03 3.81996934E+01
 4
 HOOcy (CC*CCCC) C 6 O 2 H 10 G 3E+02 2E+03 1E+03
 1
 -5.14708958E+00 1.14430443E-01-1.41643941E-04 1.06287550E-07-3.48708559E-
 11 2
 -1.34079082E+04 4.45742487E+01-5.14708958E+00 1.14430443E-01-1.41643941E-
 04 3
 1.06287550E-07-3.48708559E-11-1.34079082E+04 4.45742487E+01
 4
 O*CcyCC*CCC C 6 O 1 H 8 G 3E+02 2E+03 1E+03
 1
 2.09888530E+00 3.98562931E-02 3.00162836E-06-2.29951355E-08 9.09332753E-
 12 2

-1.03293741E+04 1.83843578E+01 2.09888530E+00 3.98562931E-02 3.00162836E-06 3
 -2.29951355E-08 9.09332753E-12 -1.03293741E+04 1.83843578E+01
 4
 CJCC*CC*COH C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -2.22733575E+00 8.71513106E-02 -8.25655441E-05 3.62951511E-08 -4.75935839E-12 2
 8.49765721E+03 3.65746862E+01 -2.22733575E+00 8.71513106E-02 -8.25655441E-05 3
 3.62951511E-08 -4.75935839E-12 8.49765721E+03 3.65746862E+01
 4
 HOCJcyCC*CCC C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -6.82528667E-01 6.63327475E-02 -4.49562608E-05 1.41682913E-08 -1.54124579E-12 2
 2.44434780E+03 3.08365672E+01 -6.82528667E-01 6.63327475E-02 -4.49562608E-05 3
 1.41682913E-08 -1.54124579E-12 2.44434780E+03 3.08365672E+01
 4
 O*CCyCCC*CC C 6 O 1 H 8 G 3E+02 2E+03 1E+03
 1
 -4.19601763E-03 4.43619084E-02 -1.05899338E-06 -2.11873966E-08 8.78733496E-12 2
 -1.00675612E+04 2.97990749E+01 -4.19601763E-03 4.43619084E-02 -1.05899338E-06 3
 -2.11873966E-08 8.78733496E-12 -1.00675612E+04 2.97990749E+01
 4
 C*CCJCC*COH C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -1.49633983E+00 8.52744700E-02 -9.11086704E-05 5.39375584E-08 -1.31543244E-11 2
 3.32016434E+03 3.32966635E+01 -1.49633983E+00 8.52744700E-02 -9.11086704E-05 3
 5.39375584E-08 -1.31543244E-11 3.32016434E+03 3.32966635E+01
 4
 HOC*cyCC*CCC C 6 O 1 H 8 G 3E+02 2E+03 1E+03
 1
 -8.51483118E+00 1.11875162E-01 -1.57709691E-04 1.27924689E-07 -4.24459208E-11 2
 -8.20723089E+03 6.21513003E+01 -8.51483118E+00 1.11875162E-01 -1.57709691E-04 3
 1.27924689E-07 -4.24459208E-11 -8.20723089E+03 6.21513003E+01
 4
 HOCOOJcyCC*CCC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 1.40593866E+01 -1.31683998E-02 1.35032220E-04 -1.58134223E-07 5.87059398E-11 2
 -1.81926413E+04 -2.80218484E+01 1.40593866E+01 -1.31683998E-02 1.35032220E-04 3
 -1.58134223E-07 5.87059398E-11 -1.81926413E+04 -2.80218484E+01
 4
 HOCOOJcyCCC*CC C 6 O 3 H 9 G 3E+02 2E+03 1E+03
 1
 1.15871108E+01 -1.34679382E-03 1.10218199E-04 -1.34476983E-07 5.03990657E-11 2
 -1.79730345E+04 -1.61450986E+01 1.15871108E+01 -1.34679382E-03 1.10218199E-04 3

-1.34476983E-07 5.03990657E-11-1.79730345E+04-1.61450986E+01
 4
 HOCJcyCCC*CC C 6 O 1 H 9 G 3E+02 2E+03 1E+03
 1
 -3.15480448E+00 7.81543535E-02-6.97702819E-05 3.78255307E-08-9.84811991E-
 12 2
 2.66395457E+03 4.27133171E+01-3.15480448E+00 7.81543535E-02-6.97702819E-
 05 3
 3.78255307E-08-9.84811991E-12 2.66395457E+03 4.27133171E+01
 4
 C*CCC (C) CJ C 6 H 11 G 3E+02 2E+03 1E+03
 1
 -1.48952815E-01 6.48328423E-02-4.03128713E-05 7.86963834E-09 1.82747940E-
 12 2
 1.62246592E+04 3.03466558E+01-1.48952815E-01 6.48328423E-02-4.03128713E-
 05 3
 7.86963834E-09 1.82747940E-12 1.62246592E+04 3.03466558E+01
 4
 Ccy (CJCCCC) C 6 H 11 G 3E+02 2E+03 1E+03
 1
 6.82868137E-01 3.10814489E-02 6.17256771E-05-1.00625842E-07 4.16568191E-
 11 2
 6.55514126E+03 2.58238354E+01 6.82868137E-01 3.10814489E-02 6.17256771E-
 05 3
 -1.00625842E-07 4.16568191E-11 6.55514126E+03 2.58238354E+01
 4
 Ccy (C*CCCC) C 6 H 10 G 3E+02 2E+03 1E+03
 1
 -8.22280328E-01 4.94754737E-02-9.48930805E-06-1.26026208E-08 5.62552511E-
 12 2
 -1.13625511E+03 2.97643682E+01-8.22280328E-01 4.94754737E-02-9.48930805E-
 06 3
 -1.26026208E-08 5.62552511E-12-1.13625511E+03 2.97643682E+01
 4
 C3H5-A C 3 H 5 G 3E+02 2E+03 1E+03
 1
 -1.91525138E+00 4.29540882E-02-4.62760161E-05 2.99612452E-08-8.36932596E-
 12 2
 1.92962957E+04 3.09666121E+01-1.91525138E+00 4.29540882E-02-4.62760161E-
 05 3
 2.99612452E-08-8.36932596E-12 1.92962957E+04 3.09666121E+01
 4
 C6H10 C 6 H 10 G 3E+02 2E+03 1E+03
 1
 2.59912596E+00 3.69133329E-02 2.40832210E-05-5.55321257E-08 2.43443210E-
 11 2
 7.58673451E+03 1.74958998E+01 2.59912596E+00 3.69133329E-02 2.40832210E-
 05 3
 -5.55321257E-08 2.43443210E-11 7.58673451E+03 1.74958998E+01
 4
 JOOcy (CCC*CC) C 5 H 7 O 2 G100.000 5000.000 832.89
 1
 8.78538562E+00 3.15799165E-02-1.31977178E-05 2.54621137E-09-1.84708440E-
 13 2
 5.91532442E+03-1.67932558E+01-3.95599844E-01 4.15548810E-02 3.02810024E-
 05 3
 -8.14356333E-08 3.97851009E-11 8.62804946E+03 3.29249158E+01
 4

-2.37931903E+00 7.06917200E-02-3.72761103E-05 1.62855007E-10 4.54207276E-
 12 2
 -2.23753357E+04 3.57095131E+01-2.37931903E+00 7.06917200E-02-3.72761103E-
 05 3
 1.62855007E-10 4.54207276E-12-2.23753357E+04 3.57095131E+01
 4
 C*CC(OH)CCC*O C 6 O 2 H 10 G 3E+02 2E+03 1E+03
 1
 5.03079238E+00 5.74924408E-02-2.26340087E-05-1.19263466E-08 9.59474038E-
 12 2
 -3.90057007E+04 8.04903780E+00 5.03079238E+00 5.74924408E-02-2.26340087E-
 05 3
 -1.19263466E-08 9.59474038E-12-3.90057007E+04 8.04903780E+00
 4
 CC*CCOOH C 4 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 2.37546515E+00 5.93219952E-02-6.85630011E-05 5.45498823E-08-1.93514672E-
 11 2
 -1.27315463E+04 1.64206840E+01 2.37546515E+00 5.93219952E-02-6.85630011E-
 05 3
 5.45498823E-08-1.93514672E-11-1.27315463E+04 1.64206840E+01
 4
 C*CC(C)OOH C 4 O 2 H 8 G 3E+02 2E+03 1E+03
 1
 -1.72088932E+00 8.57690269E-02-1.16471261E-04 9.10896446E-08-2.96684965E-
 11 2
 -1.34542610E+04 3.21625371E+01-1.72088932E+00 8.57690269E-02-1.16471261E-
 04 3
 9.10896446E-08-2.96684965E-11-1.34542610E+04 3.21625371E+01
 4
 CC*CCOJ C 4 O 1 H 7 G 3E+02 2E+03 1E+03
 1
 6.56512602E+00 1.46164800E-02 2.09267514E-05-2.71097024E-08 8.93552423E-
 12 2
 4.99755370E+03-1.75803022E+00 6.56512602E+00 1.46164800E-02 2.09267514E-
 05 3
 -2.71097024E-08 8.93552423E-12 4.99755370E+03-1.75803022E+00
 4
 HOcyCCJCCPCC C 6 O 3 H 11 G 3E+02 2E+03 1E+03
 1
 -1.32892986E+00 9.30930732E-02-8.34329623E-05 5.53580282E-08-1.99781552E-
 11 2
 -2.54045504E+04 3.40126454E+01-1.32892986E+00 9.30930732E-02-8.34329623E-
 05 3
 5.53580282E-08-1.99781552E-11-2.54045504E+04 3.40126454E+01
 4
 CH2CHOO C 2 H 3 O 2 G100.000 5000.000 2061.90
 1
 -1.23554713E+01 3.19636708E-02-8.47059615E-06-4.40031992E-10 1.06897398E-
 13 2
 2.31221484E+04 1.07303923E+02 2.08408870E+00 2.73787874E-02-2.21780699E-
 05 3
 9.50235684E-09-1.76671068E-12 1.21875750E+04 1.51163354E+01
 4
 END

REACTIONS

!*****
 !*** 1,5-hexadiene pyrolysis and oxidation mechanism ***
 !*****

C2H3+C*cy(CCC*CCC)=C2H4+C*cy(CCC*CCJC) 6572.5	1.57E13	0.000
C2H3+C*cy(CCC*CCC)=C2H4+CJcy(C*CC*CCC) 6572.5	1.57E13	0.000
C2H3+C*cy(CCC*CCC)=C2H4+CJcy(C*CCC*CC) 7361.2	1.61E13	0.000
C2H3+Ccy(CC*CCC*C)=C2H4+C7H9r_olef_1 12882.1	3.01E13	0.000
C2H3+Ccy(CC*CCC*C)=C2H4+Ccy(C*CCJCC*C) 3847.9	3.90E12	0.000
C2H3+Ccy(CC*CCC*C)=C2H4+Ccy(CCJC*CC*C) 5114.6	2.60E13	0.000
C2H3+C7H10_R6=C2H4+C*cy(CC*CCCJC) 10587.7	2.15E13	0.000
C2H3+C7H10_R6=C2H4+CJcy(C*CC*CCC) 6142.3	1.20E13	0.000
C2H3+C7H10_R6=C2H4+C7H9r_olef 6931.0	1.23E13	0.000
C2H3+Ccy(C*CC*CCC)=C2H4+CJcy(C*CC*CCC) 9034.2	7.46E12	0.000
C2H3+Ccy(C*CC*CCC)=C2H4+Ccy(C*CCCJC*C) 7361.2	1.61E13	0.000
C2H3+Ccy(C*CC*CCC)=C2H4+Ccy(CJCC*CC*C) 7361.2	1.61E13	0.000
C2H3+Ccy(C*CCC*CC)=C2H4+CJcy(C*CCC*CC) 9034.2	7.46E12	0.000
C2H3+Ccy(C*CCC*CC)=C2H4+Ccy(C*CCCJC*C) 5114.6	1.73E13	0.000
C2H3+Ccy(C*CCC*CC)=C2H4+Ccy(CJCC*CC*C) 5114.6	1.73E13	0.000
C2H3+Ccy(C*CCCC*C)=C2H4+C7H9r_olef 9034.2	7.46E12	0.000
C2H3+Ccy(C*CCCC*C)=C2H4+Ccy(C*CCCJC*C) 7361.2	1.61E13	0.000
C2H3+Ccy(C*CCCC*C)=C2H4+Ccy(C*CCJCC*C) 7361.2	1.61E13	0.000
C2H3+Ccy(CC*CC*CC)=C2H4+Ccy(CCJC*CC*C) 7361.2	1.61E13	0.000
C2H3+Ccy(CC*CC*CC)=C2H4+Ccy(CJCC*CC*C) 5903.3	5.34E12	0.000
C2H5+C*cy(CCC*CCC)=C2H6+C*cy(CCC*CCJC) 12667.0	2.63E12	0.000
C2H5+C*cy(CCC*CCC)=C2H6+CJcy(C*CC*CCC) 12667.0	2.63E12	0.000
C2H5+C*cy(CCC*CCC)=C2H6+CJcy(C*CCC*CC) 13455.7	2.69E12	0.000
C2H5+Ccy(CC*CCC*C)=C2H6+C7H9r_olef_1 18976.6	4.98E12	0.000
C2H5+Ccy(CC*CCC*C)=C2H6+Ccy(C*CCJCC*C) 9942.4	6.52E11	0.000
C2H5+Ccy(CC*CCC*C)=C2H6+Ccy(CCJC*CC*C) 11209.1	2.89E12	0.000

C2H5+C7H10_R6=C2H6+C*cy (CC*CCCJC) 16682.2	3.51E12	0.000
C2H5+C7H10_R6=C2H6+CJcy (C*CC*CCC) 12236.8	2.00E12	0.000
C2H5+C7H10_R6=C2H6+C7H9r_Olef 13025.5	2.05E12	0.000
C2H5+Ccy (C*CC*CCC) =C2H6+CJcy (C*CC*CCC) 15128.7	1.25E12	0.000
C2H5+Ccy (C*CC*CCC) =C2H6+Ccy (C*CCCJC*C) 13455.7	2.69E12	0.000
C2H5+Ccy (C*CC*CCC) =C2H6+Ccy (CJCC*CC*C) 13455.7	2.69E12	0.000
C2H5+Ccy (C*CCC*CC) =C2H6+CJcy (C*CCC*CC) 15128.7	1.25E12	0.000
C2H5+Ccy (C*CCC*CC) =C2H6+Ccy (C*CCCJC*C) 11209.1	2.89E12	0.000
C2H5+Ccy (C*CCC*CC) =C2H6+Ccy (CJCC*CC*C) 11209.1	2.89E12	0.000
C2H5+Ccy (C*CCCC*C) =C2H6+C7H9r_Olef 15128.7	1.25E12	0.000
C2H5+Ccy (C*CCCC*C) =C2H6+Ccy (C*CCCJC*C) 13455.7	2.69E12	0.000
C2H5+Ccy (C*CCCC*C) =C2H6+Ccy (C*CCJCC*C) 13455.7	2.69E12	0.000
C2H5+Ccy (CC*CC*CC) =C2H6+Ccy (CCJC*CC*C) 13455.7	2.69E12	0.000
C2H5+Ccy (CC*CC*CC) =C2H6+Ccy (CJCC*CC*C) 11997.8	8.92E11	0.000
C3H5-A+C*cy (CCC*CCC) =C3H6+C*cy (CCC*CCJC) 23637.1	3.49E13	0.000
C3H5-A+C*cy (CCC*CCC) =C3H6+CJcy (C*CC*CCC) 23637.1	3.49E13	0.000
C3H5-A+C*cy (CCC*CCC) =C3H6+CJcy (C*CCC*CC) 24425.8	3.58E13	0.000
C3H5-A+Ccy (CC*CCC*C) =C3H6+C7H9r_Olef_1 29946.7	5.53E13	0.000
C3H5-A+C7H10_R6=C3H6+C*cy (CC*CCCJC) 27652.3	3.89E13	0.000
C3H5-A+C7H10_R6=C3H6+CJcy (C*CC*CCC) 23206.9	2.66E13	0.000
C3H5-A+C7H10_R6=C3H6+C7H9r_Olef 23995.6	2.73E13	0.000
C3H5-A+Ccy (C*CC*CCC) =C3H6+CJcy (C*CC*CCC) 26098.8	1.66E13	0.000
C3H5-A+Ccy (C*CCC*CC) =C3H6+CJcy (C*CCC*CC) 26098.8	1.66E13	0.000
C3H5-A+Ccy (C*CCCC*C) =C3H6+C7H9r_Olef 26098.8	1.66E13	0.000
CH3+C*cy (CCC*CCC) =CH4+C*cy (CCC*CCJC) 11376.4	1.62E13	0.000
CH3+C*cy (CCC*CCC) =CH4+CJcy (C*CC*CCC) 11376.4	1.62E13	0.000
CH3+C*cy (CCC*CCC) =CH4+CJcy (C*CCC*CC) 12165.1	1.66E13	0.000
CH3+Ccy (CC*CCC*C) =CH4+C7H9r_Olef_1 17686.0	3.10E13	0.000
CH3+C7H10_R6=CH4+C*cy (CC*CCCJC) 15391.6	2.22E13	0.000

CH3+C7H10_R6=CH4+CJcy (C*CC*CCC)		1.23E13	0.000	
10946.2				
CH3+C7H10_R6=CH4+C7H9r_Olef		1.26E13	0.000	11734.9
CH3+Ccy (C*CC*CCC)=CH4+CJcy (C*CC*CCC)		7.68E12	0.000	
13838.1				
CH3+Ccy (C*CCC*CC)=CH4+CJcy (C*CCC*CC)		7.68E12	0.000	
13838.1				
CH3+Ccy (C*CCCC*C)=CH4+C7H9r_Olef		7.68E12	0.000	
13838.1				
C6H11Or_Olef_23=C6H11Or_Olef_25	3.70E10	0.000	28345.4	
C6H9Or_Olef_18=C6H8O_Olef_15+H	1.17E10	1.000	18548.8	
C6H11Or_Olef_46=C6H11Or_Olef_48	7.40E10	0.000	16084.7	
C6H11Or_Olef_31=C2H3+C4H8O_Olef_1	4.20E13	0.000	36351.9	
C6H11Or_Olef_3=C6H11Or_Olef_13	6.87E9	0.000	29636.0	
C6H9Or_Olef=C2H3+C4H6O_Olef_1	2.35E14	0.000	45290.5	
C6H9Or_Olef_13=CH3CHCHCHO+C2H3	8.10E14	0.000	23890.4	
C6H11Or_Olef_25=C3H6+SC3H4OH4	4.20E13	0.000	36351.9	
C6H11Or_Olef_32=C6H11Or_Olef_33	6.00E11	0.000	34463.8	
C3H5Or_Olef+C6H10=IC3H5OH+C6H9-A	7.15E13	0.000	24425.8	
C4H5-N+C6H10=C4H6+C6H9-A	3.22E13	0.000	7361.2	
C6H11Or_Olef_42=C6H11Or_Olef_40	9.16E9	0.000	15176.5	
C6H9Or_Olef_9=C6H8O_Olef_9+H3	5.2E10	1.000	18548.8	
CC*CCCJ=C2H4+C3H5-S	6.93E13	0.000	36543.1	
C6H9Or_Olef_12=C*CC(*O)CC*C+H	5.87E9	1.000	18548.8	
C6H11r_Olef_1=C6H11r_Olef_7	1.11E11	0.000	32049.9	
C4H5-N+C6H10_Olef_3=C4H6+C6H9-A	7.46E12	0.000	9034.2	
C6H9Or_Olef_5=>C5H9r_Olef_2+CO	3.30E12	0.620	17298.8	
PC2H4OH+C6H10=C2H5OH+C6H9-A	5.38E12	0.000	13455.7	
C4H71-3+C6H10_Olef_3=C4H8-2+C6H9-A	8.29E12	0.000	26098.8	
H+C6H10_Olef_6=H2+C*CCJC*CC	1.46E14	0.000	9177.6	
C6H11Or_Olef_35=C6H10_Olef_3+OH	3.00E13	0.000	26799.1	
O2+C*cy (CC*CCC)=HO2+C*cy (CCJCC*C)	2.00E13	0.000	35343.2	
C6H11Or_Olef_18=C6H11Or_Olef_16	1.37E10	0.000	18665.9	
C5H7r_Olef=>C2H2+C3H5-S	3.52E13	0.000	30711.5	
C5H7r_Olef=C*CC*CCJ	5.55E10	0.000	9727.3	
C6H11Or_Olef_55=C2H3+C4H8O_Olef_2	4.20E13	0.000	36351.9	
C6H9O2r_Olef_15=C*CC*CC*C+HO2	3.16E10	0.637	27578.2	
C4H71-3+C6H10_Olef_6=C4H8-1+C*CCJC*CC	2.14E13	0.000	27508.9	
C6H9Or_Olef_22=C6H8O_Olef_18+H	1.76E10	1.000	18548.8	
C6H11=Ccy (CCCJCC)	3.74E10	0.000	16538.8	
C6H9r_Olef=cy (C*CCJCCC)	1.04E10	0.000	7648.0	
C3H5-A+C*CCC*C=C3H6+C*CC*CCJ3	8.5E13	0.000	22179.2	
C6H11O3r_3=C6H11O3r_1	2.91E12	-0.230	22298.7	
HO2+C6H10=H2O2+C6H9-A	1.02E-1	4.400	13546.5	
C3H5Or_Olef+C6H10_Olef_3=IC3H5OH+C*CCJC*CC	3.85E13	0.000	22179.2	
C6H11Or_Olef_54=C6H11Or_Olef_52	7.20E12	0.000	43020.0	
C6H11Or_Olef_32=C6H11Or_Olef_34	3.00E11	0.000	31691.4	
H+C6H10O_Olef_9=H2+C6H9Or_Olef_3	7.15E5	2.400	1577.4	
O2+C6H10_Olef_3=HO2+C6H9-A	3.00E13	0.000	38371.0	
C4H71-3+C6H10=C4H8-1+C6H9-A	4.62E13	0.000	25835.9	
O2+C*cy (CCC*CC)=HO2+C*cy (CCJC*CC)	4.00E13	0.000	25116.2	
C6H10_Olef_1+H=C6H11r_Olef_15	0.3E13	0.000	2748.5	
C6H9Or_Olef_13=C6H8O_Olef_14+H	1.76E10	1.000	18548.8	
C6H9O2r_Olef_4=C6H9O2r_Olef_18	7.68E12	-0.130	34358.6	
C6H11Or_Olef_22=C2H4+C4H7Or_Olef_2	1.51E13	0.000	20745.2	
C6H11O2r_1=C*CCCcy (COC)+OH	4.56E8	1.290	9889.8	
O2+C*CCJC*CC=C6H9O2r_Olef_4	2.90E7	1.590	1080.3	

DUP

C4H5-N+C6H10_olef_3=C4H6+C*CCJC*CC 1.73E13 0.000 5114.6
C6H9O2r_olef_6=C6H9O2r_olef_16 1.34E7 1.290 14239.6
C6H11Or_olef_46=C6H11Or_olef_49 4.80E12 0.000 52484.4
C6H11r_olef_4=Ccy(CCJCCC) 7.48E10 0.000 19167.8
C*CC*CC*C+H=C6H9r_olef 1.57E14 0.000 5951.1
DUP
O2+Ccy(CC*CC*C)=HO2+CJcy(CC*CC*C) 3.00E13 0.000 52666.1
C6H9Or_olef_13=C3H5-S+C2H3CHO 8.10E14 0.000 23890.4
C6H9O4r_olef_1=C6H8O3_olef_3+OH 4.91E0 2.655 18214.2
C6H9Or_olef_22=C5H6O_olef_1+CH3 9.00E13 0.220 14098.6
C6H11Or_olef_54=CH3+C5H8O_olef_7 4.27E13 0.000 30520.3
O2+C*CCJC*CC=C6H9O2r_olef_112.90E7 1.590 1080.3
DUP
C6H11r_olef=C2H3+C4H8-1 4.20E13 0.000 36351.9
OH+C6H8O_olef_9=H2O+C6H7Or_olef 6.13E4 2.700 -4588.8
O2+C6H9O2r_olef_16=C6H9O4r_olef_1 2.90E7 1.590 1080.3
DUP
C4H5-N+C*CC*CC=C4H6+C*CC*CCJ7.46E12 0.000 9034.2
H+C6H10_olef_3=H2+C6H9-A 7.28E13 0.000 9177.6
C6H9Or_olef_9=C5H7r_olef+CH2O 8.10E14 0.000 23890.4
C6H11Or_olef_39=CH3+C*CC*CCOH 2.39E14 0.000 39458.9
C*cy(CC*CCC)+H=C6H9r_R5_1 5.61E13 0.000 2294.4
O2+CPC*CCJC*C=C6H9O4r_olef_10 2.90E7 1.590 1080.3
DUP
C6H11Or_olef_46=C2H5+C4H6O_olef_1 1.72E14 0.000 37379.6
!O2+C6H10_olef_3=HO2+C*CCJC*CC 2.00E13 0.000 18583.7
C6H11Or_olef_37=C4H71-3+C2H3OH 5.92E13 0.000 21844.6
C6H11Or_olef_32=C6H11Or_olef_37 4.58E9 0.000 25716.4
!H+C*CC*CC=H2+C*CC*CCJ 7.28E13 0.000 9177.6
C*CCCCJCP=C6H10+HO2 1.83E10 0.790 15099.6
C3H5Or_olef+C6H10_olef_1=IC3H5OH+C*CCJC*CC 3.58E13 0.000 24425.8
!C3H5-A+C6H10=C3H6+C6H9-A 7.15E13 0.000 24425.8
C3H5-S+C*CC*CC=C3H6+C*CC*CCJ7.46E12 0.000 9034.2
O2+C*CCJC*CC=C6H9O2r_olef_6 2.90E7 1.590 1080.3
DUP
O2+Ccy(C*CC*CC)=HO2+C*cy(CCJC*CC) 3.00E13 0.000 32844.7
C6H11Or_olef_32=C6H11Or_olef_35 3.70E10 0.000 28345.4
CPC*CCJC*C=C6H8O_olef_7+OH 2.28E8 1.290 9889.8
C4H71-1+C6H10_olef_3=C4H8-1+C*CCJC*CC 1.73E13 0.000 5114.6
C6H11r_olef_7=C2H4+C4H71-1 6.93E13 0.000 36543.1
HO2+C6H10_olef_3=H2O2+C6H9-A7.68E-2 4.400 13546.5
O2+Ccy(C*CC*CC)=HO2+C*cy(CCJC*CC) 3.00E13 0.000 39114.2
C4H71-1+C6H10_olef_3=C4H8-1+C6H9-A 7.46E12 0.000 9034.2
SC2H4OH+C6H10=C2H5OH+C6H9-A 4.65E13 0.000 16849.5
C3H5Or_olef_1+C6H10_olef_1=SC3H5OH+C6H9r_olef 2.64E13 0.000
29946.7
C6H11Or_olef_14=C6H11Or_olef_22 7.20E12 0.000 54778.8
C6H11r_olef_7=C6H11r_olef_7 6.87E9 0.000 18665.9
C6H11Or_olef_14=CH3+C5H8O_olef_5 2.39E14 0.000 39458.9
H+C6H10_olef_1=H2+C6H9r_olef 2.87E14 0.000 12499.7
C6H11Or_olef_3=C4H6+SC2H4OH 2.90E14 0.000 33866.3 ! RDB /2
C6H11Or_olef_28=C4H8-1+C2H3Or_olef 4.27E13 0.000 30520.3
SC2H4OH+C6H10_olef_1=C2H5OH+C6H9r_olef 3.98E13 0.000 22370.4
CH2OH+C6H10_olef_3=CH3OH+C*CCJC*CC 1.31E13 0.000 14411.7
C6H11Or_olef_35=C3H5-S+C3H5OH 4.20E13 0.000 36351.9
C6H9r_R5_5=CH3+C5H6 2.59E13 0.000 27126.5
C*CCJC*CC+HO2=C6H10O2_olef_15 3.35E10 0.600 -2105.6
DUP

C6H10O2_olef_8=>C6H9Or_olef_13+OH 1.59E20 -1.500 42857.5
C6H11r_olef_4=C6H11r_olef_1 4.80E12 0.000 36877.7
Ccy(CC*CC*C)+H=C6H9r_R5_5 1.64E14 0.000 5377.5
DUP
HO2+C5H6O_olef_1=H2O2+C*CC*CCJ*O 1.18E-4 4.900 3680.6
Ccy(C*CCC*C)+H=C6H9r_R5 8.20E13 0.000 5377.5
CH3+C*CCC*C=CH4+C*CC*CCJ 1.78E13 0.000 9918.5
NC3H7+C*CC*CC=C3H8+C*CC*CCJ 8.25E11 0.000 14459.5
C6H11Or_olef_1=C6H11Or_olef_31 4.80E12 0.000 40773.4
C3H5-A+C6H10_olef_1=C3H6+C*CCJC*CC 3.58E13 0.000 24425.8
C6H11Or_olef_18=C2H4+C4H7Or_olef_3 6.93E13 0.000 36543.1
C6H9O4r_olef_7=C6H8O3_olef_1+OH 4.47E6 1.290 14239.6
C3H5Or_olef+C6H10_olef_1=IC3H5OH+C6H9r_olef 5.73E13 0.000 29946.7
C6H9O2r_olef_16=C6H8O_olef+OH 2.28E8 1.290 9889.8
C2H3+C6H10_olef_1=C2H4+C6H9r_olef 3.01E13 0.000 12882.1
C6H11Or_olef_54=C4H8-1+C2H2OH 4.20E13 0.000 36351.9
OH+C6H10_olef_1=H2O+C*CCJC*CC 1.50E5 2.400 -932.1
NC3H7+C6H10_olef_3=C3H8+C6H9-A 8.25E11 0.000 14459.5
C*CCCCJCOH=C6H11Or_olef_32 4.80E12 0.000 37499.1
C*CCCCCJ=CJcy(CCCCC) 5.60E10 0.000 9804.7
C6H10O2_olef_5=>C6H9Or_olef_18+OH 1.59E20 -1.500 42857.5
C*cy(CCC*CC)+H=C6H9r_R5_7 1.35E14 0.000 4803.9
C*CCJC*CC+HO2=C6H10O2_olef_23.35E10 0.600 -2105.6
DUP
C6H11O2r_1=C6H10+HO2 3.66E10 0.790 15099.6
C6H7Or_olef=>C5H7r_olef+CO 3.30E12 0.620 17298.8
NC3H7+C6H10=C3H8+C6H9-A 3.56E12 0.000 12786.5
C6H11Or_olef_34=C6H11Or_olef_40 7.40E10 0.000 28560.5
NC3H7+C6H10_olef_1=C3H8+C6H9r_olef 3.30E12 0.000 18307.4
O2+C*CCJC*CC=C6H9O2r_olef_112.90E7 1.590 1080.3
DUP
Ccy(C*CC*CC)+H=C6H9r_R5_1 6.11E13 0.000 3704.5
C6H11Or_olef_16=C6H10_olef_1+OH 6.00E13 0.000 26799.1
C*CCJC*CC+HO2=C6H10O2_olef_23.35E10 0.600 -2105.6
DUP
C*CCJC*CC+HO2=C6H10O2_olef_83.35E10 0.600 -2105.6
DUP
C3H5Or_olef_1+C6H10_olef_1=C3H5OH+C*CCJC*CC 1.66E13 0.000 12165.1
H+C*CCCC*O=H2+C6H9Or_olef_67.15E5 2.400 1577.4
C6H11Or_olef_5=C6H10_olef_6+OH 3.00E13 0.000 26799.1
C6H10_olef_3+H=C6H11r_olef 6.75E13 0.000 4803.9
C*CCCCJ=cy(CJCCCC) 1.04E10 0.000 10372.6
C6H9Or_olef_2=>CC*CCCJ+CO 3.30E12 0.620 17298.8
Ccy(CCJCCC)=CH3+cy(C*CCCC) 4.66E13 0.000 30424.7
C*CCCCJ=C4H71-4+C2H4 5.05E13 0.000 28632.2
C6H11Or_olef_3=C6H11Or_olef_4 2.40E12 0.000 57264.4
C6H11Or_olef_1=C4H71-4+C2H3OH 5.40E13 0.000 27604.5
C*CC*CC*C+H=C6H9r_olef 1.57E14 0.000 5951.1
DUP
O2+C*CCJC*CC=C6H9O2r_olef_112.90E7 1.590 1080.3
DUP
C6H11Or_olef_27=C6H11Or_olef_28 4.80E12 0.000 40104.2
O2+Ccy(CC*CC*C)=HO2+Ccy(CJC*CC*C) 1.00E13 0.000 28672.7
SC2H4OH+C6H10_olef_6=C2H5OH+C*CCJC*CC 2.16E13 0.000 18522.5
C6H11r_olef_2=C3H5-S+C3H6 4.20E13 0.000 36351.9
C6H11Or_olef_13=C6H11Or_olef_5 4.80E12 0.000 37546.9
O2+C6H9O2r_olef_16=C6H9O4r_olef_7 2.90E7 1.590 1080.3
DUP

O2+C*CCJC*CC=C6H9O2r_Olef_112.90E7 1.590 1080.3
DUP
!O2+cy(C*CCC*CC)=HO2+cy(C*CC*CCJC) 2.00E13 0.000 26870.4 ! RDB
/2
C4H5-N+C6H10_Olef_1=C4H6+C*CCJC*CC 1.61E13 0.000 7361.2
C6H9Or_Olef_12=C3H5-A+C2H3CHO 3.00E13 0.220 14098.6
O2+C6H9O2r_Olef_16=C6H9O4r_Olef_7 2.90E7 1.590 1080.3
DUP
CH3+C6H10O_Olef_6=CH4+C6H9Or_Olef_2 5.00E0 3.600 4328.3
C*CCJCCC=C6H11r_Olef_2 3.70E10 0.000 28345.4
C6H11Or_Olef_3=C6H11Or_Olef_7 1.85E10 0.000 33125.4
Ccy(C*CC*CC)+H=C6H9r_R5_2 9.27E13 0.000 4780.0
OH+C6H10_Olef_3=H2O+C6H9-A 7.80E5 2.300 -1362.3
C6H9O2r_Olef_4=C*CC*CC*C+HO28.66E9 0.930 29799.3
C3H5-A+C6H10_Olef_3=C3H6+C6H9-A 1.66E13 0.000 26098.8
C6H11O3r_7=C5H9O2r_Olef+CH2O3.00E13 0.220 14098.6
C*cy(CC*CCC)+H=CJcy(CC*CCC) 2.53E13 0.000 6739.8
C6H10_Olef_1+H=C6H11r_Olef 8.20E13 0.000 5377.5
O2+CPC*CCJC*C=C6H9O4r_Olef_13 2.90E7 1.590 1080.3
DUP
!C6H11O3r_1=C4H71-4+C2H4O3 3.00E13 0.220 14098.6
HO2+C6H10O_Olef_6=H2O2+C6H9Or_Olef_2 1.18E-4 4.900 3680.6
C6H9O2r_Olef_18=C*CC*CC*C+HO2 3.66E10 0.790 15099.6
C5H9O2r_Olef=C*CCCC*O+OH 1.00E12 0.000 0.0
C6H11Or_Olef_39=C6H11Or_Olef_44 7.20E12 0.000 54778.8
!O2+cy(C*CC*CCC)=HO2+cy(C*CC*CCJC) 2.00E13 0.000 27350.6 ! RDB
/2
O2+C6H9O2r_Olef_16=C6H9O4r_Olef_1 2.90E7 1.590 1080.3
DUP
OH+C6H8O_Olef_15=H2O+C6H7Or_Olef_1 6.13E4 2.700 -4588.8
C4H71-4+C6H10_Olef_6=C4H8-1+C*CCJC*CC 2.49E12 0.000 15128.7
!O2+C6H10_Olef_6=HO2+C*CCJC*CC 6.00E13 0.000 24163.4
C6H10O2_Olef_15=>C6H9Or_Olef_9+OH 1.59E20 -1.500 42857.5
C4H71-3+C*CCC*C=C4H8-1+C*CC*CCJ 2.49E13 0.000 23589.3
C6H11Or_Olef_48=C3H6+C3H5Or_Olef_2 4.20E13 0.000 36351.9
H+C6H10=H2+C6H9-A 1.30E14 0.000 7074.4 ! RDB /2
O2+C6H9O2r_Olef_16=C6H9O4r_Olef_1 2.90E7 1.590 1080.3
DUP
OH+C*CCCC*O=H2O+C5H7Or_Olef 6.13E4 2.700 -4588.8
C3H5Or_Olef_1+C6H10_Olef_6=SC3H5OH+C*CCJC*CC 1.66E13 0.000 26098.8
C4H71-1+C6H10=C4H8-1+C6H9-A 3.22E13 0.000 7361.2
C6H11Or_Olef_5=C6H11Or_Olef_14 3.00E11 0.000 41538.2
O2+C6H9-A=C6H9O2r_Olef_15 2.90E7 1.590 1080.3
DUP
C6H11Or_Olef_16=C4H71-1+C2H3OH 7.41E13 0.000 35515.4
C3H5-S+C6H10_Olef_3=C3H6+C6H9-A 7.46E12 0.000 9034.2
O2+C6H9-A=C6H9O2r_Olef 2.90E7 1.590 1080.3
DUP
C6H11Or_Olef_3=C6H11Or_Olef_5 3.00E11 0.000 32121.6
C6H11Or_Olef_42=C6H11Or_Olef_39 7.40E10 0.000 14148.8
C6H11Or_Olef_39=C6H11Or_Olef_46 6.00E11 0.000 32862.5
!O2+C*CCCCJCOH=C6H11O3r_5 3.02E15 -0.920 -129.1 ! RDB Disabled
Waddington
!DUP
C3H5-S+C6H10_Olef_3=C3H6+C*CCJC*CC 1.73E13 0.000 5114.6
!O2+C6H11Or_Olef_1=C6H11O3r_3 5.20E11 0.230 -1579.8
!DUP
C6H11Or_Olef_28=CH3+C5H8O_Olef_6 4.27E13 0.000 30520.3

C6H11Or_olef_13=C4H71-3+C2H3OH 1.61E13 0.000 19717.5
OH+C*CCCC*O=H2O+C6H9Or_olef_6 6.13E4 2.700 -4588.8
C3H5-S+C6H10_olef_6=C3H6+C*CCJC*CC 1.49E13 0.000 9034.2
C3H5Or_olef_1+C6H10_olef_6=C3H5OH+C*CCJC*CC 1.54E13 0.000 13838.1
C2H3+C*CC*CC=C2H4+C*CC*CCJ 7.46E12 0.000 9034.2
C6H10_olef_3+H=C6H11r_olef_25.56E13 0.000 3847.9
DUP
C6H9Or_olef_3=>C*CCJCC+CO 3.30E12 0.620 17298.8
C2H5+C6H10_olef_6=C2H6+C*CCJC*CC 2.49E12 0.000 15128.7
H+C6H10O_olef_6=H2+C6H9Or_olef_2 7.15E5 2.400 1577.4
O2+C*CCJC*CC=C6H9O2r_olef_6 2.90E7 1.590 1080.3
DUP
C2H3+C6H10=C2H4+C6H9-A 3.22E13 0.000 7361.2
C3H5-S+C*CCC*C=C3H6+C*CC*CCJ 1.73E13 0.000 5114.6
C2H5+C6H10=C2H6+C6H9-A 5.38E12 0.000 13455.7
C6H11Or_olef_37=C6H11Or_olef_34 4.80E12 0.000 40271.5
C6H10O2_olef_2=>C6H9Or_olef_22+OH 1.59E20 -1.500 42857.5
O2+C6H9O2r_olef_16=C6H9O4r_olef_7 2.90E7 1.590 1080.3
DUP
O2+CPC*CCJC*C=C6H9O4r_olef_13 2.90E7 1.590 1080.3
DUP
C6H11Or_olef_42=C2H4+C4H7Or_olef_4 6.93E13 0.000 36543.1
C2H5+C*CCC*C=C2H6+C*CC*CCJ 2.89E12 0.000 11209.1
C6H11Or_olef_23=C6H11Or_olef_26 4.80E12 0.000 52484.4
O2+Ccy(C*CC*CC)=HO2+Ccy(CJC*CC*C) 2.00E13 0.000 32253.9
C3H5-A+C6H10_olef_1=C3H6+C6H9r_olef 5.50E13 0.000 29946.7
O2+C*CCJC*CC=C6H9O2r_olef_6 2.90E7 1.590 1080.3
DUP
CH3+C*CCCC*O=CH4+C6H9Or_olef_6 5.00E0 3.600 4328.3
C6H7Or_olef_1=>CJ*CCC*C+CO 3.30E12 0.620 17298.8
C6H11O3r_5=C6H10O_olef_4+HO2 5.77E9 0.930 29799.3
C3H5-S+C6H10_olef_1=C3H6+C6H9r_olef 3.01E13 0.000 12882.1
C6H9O2r_olef_18=C6H8O_olef_7+OH 4.56E8 1.290 9889.8
C6H9Or_olef_22=C4H5-N+CH3CHO 8.10E14 0.000 23890.4
C2H4+C4H5-N=C6H9r_olef 5.56E12 0.000 6644.2
DUP
C2H4+C4H5-N=C6H9r_olef 5.56E12 0.000 6644.2
DUP
C2H2+C4H5-N=C*CC*CC*CJ 1.42E13 0.000 7361.2
DUP
C2H2+C4H5-N=C*CC*CC*CJ 1.42E13 0.000 7361.2
DUP
C4H71-1+C*CCC*C=C4H8-1+C*CC*CCJ 1.73E13 0.000 5114.6
C6H9O4r_olef_10=C6H8O3_olef_10+OH 8.94E6 1.290 14239.6
C6H11Or_olef_31=C5H8O_olef_7+CH3 4.57E13 0.000 29492.6
C2H5+C6H10_olef_3=C2H6+C6H9-A 1.25E12 0.000 15128.7
OH+C6H10O_olef_11=H2O+C6H9Or_olef_5 6.13E4 2.700 -4588.8
OH+C6H10=H2O+C6H9-A 1.50E5 2.400 -932.1 !RDB/2
C6H11Or_olef_40=C4H71-1+C2H3OH 2.72E14 0.000 37642.5
C*CCCCJ=C6H11r_olef 4.80E12 0.000 40104.2
C6H9Or_olef_18=CJ*CCC*C+CH2O 2.70E14 0.000 23890.4
HO2+C6H10O_olef_11=H2O2+C6H9Or_olef_5 1.18E-4 4.900 3680.6
O2+C6H10_olef_1=HO2+C6H9r_olef 3.00E13 0.000 53049.0
C6H9O2r_olef=CPC*CCJC*C 8.94E6 1.290 14239.6
H+C*CCCC*O=H2+C5H7Or_olef 7.15E5 2.400 1577.4
C6H9r_olef=CJcy(CC*CCC) 2.80E10 0.000 9780.8
C6H10_olef_6+H=C6H11r_olef_21.64E14 0.000 5377.5
DUP

C6H11Or_Olef_23=C6H11Or_Olef_22 6.87E9 0.000 29205.8
C6H11r_Olef=C*CCC*C+CH3 4.27E13 0.000 30520.3
HO2+C6H10O_Olef_9=H2O2+C6H9Or_Olef_3 1.18E-4 4.900 3680.6
C6H11Or_Olef_46=C6H11Or_Olef_44 1.37E10 0.000 16945.1
C6H9Or_Olef_12=C*CCC*O+C2H3 2.70E14 0.000 23890.4
C6H11Or_Olef_14=C6H11Or_Olef_23 9.00E11 0.000 34535.5
C3H5Or_Olef_1+C6H10_Olef_1=SC3H5OH+C*CCJC*CC 1.79E13 0.000 24425.8
O2+CPC*CCJC*C=C6H9O4r_Olef_13 2.90E7 1.590 1080.3
DUP
C6H11Or_Olef_46=C6H11Or_Olef_52 9.00E11 0.000 37953.2
CH3+C6H10_Olef_3=CH4+C*CCJC*CC 1.78E13 0.000 9918.5
SC2H4OH+C6H10_Olef_3=C2H5OH+C*CCJC*CC 2.50E13 0.000 14602.9
C6H11Or_Olef_18=C6H11Or_Olef_14 3.70E10 0.000 22155.3
CH3+C*CCCC*O=CH4+C5H7Or_Olef 5.00E0 3.600 4328.3
C4H71-3+C6H10_Olef_3=C4H8-1+C*CCJC*CC 2.49E13 0.000 23589.3
C4H71-4+C6H10_Olef_1=C4H8-1+C*CCJC*CC 2.69E12 0.000 13455.7
HO2+C*CC*CC=H2O2+C*CC*CCJ 7.68E-2 4.400 13546.5
O2+C6H9O2r_Olef_16=C6H9O4r_Olef_1 2.90E7 1.590 1080.3
DUP
C4H71-4+C6H10_Olef_3=C4H8-1+C*CCJC*CC 2.89E12 0.000 11209.1
C6H9Or_Olef_6=>C*CCCCJ+CO 3.30E12 0.620 17298.8
O2+C*CCJC*CC=C6H9O2r_Olef_4 2.90E7 1.590 1080.3
DUP
C*CCJC*CC+HO2=C6H10O2_Olef_23.35E10 0.600 -2105.6
DUP
HO2+C*CCCC*O=H2O2+C5H7Or_Olef 1.18E-4 4.900 3680.6
CH3+C6H8O_Olef_9=CH4+C6H7Or_Olef 5.00E0 3.600 4328.3
O2+C*CCJC*CC=C6H9O2r_Olef_4 2.90E7 1.590 1080.3
DUP
C6H11Or_Olef_55=C*CCC*C+CH2OH 6.65E13 0.000 26935.3
C4H5-N+C6H10_Olef_6=C4H6+C*CCJC*CC 1.49E13 0.000 9034.2
C6H11Or_Olef_16=C6H11Or_Olef_5 7.40E10 0.000 14148.8
C6H11Or_Olef_44=C2H4+C4H7Or_Olef_7 1.51E13 0.000 20745.2
C6H11Or_Olef_13=C6H10_Olef_3+OH 6.00E13 0.000 26799.1
H+C6H10_Olef_1=H2+C*CCJC*CC 1.59E14 0.000 7361.2
OH+C5H6O_Olef_1=H2O+C*CC*CCJ*O 6.13E4 2.700 -4588.8
C6H11Or_Olef_5=C5H8O_Olef_3+CH3 2.56E14 0.000 38431.2
C6H11Or_Olef_52=C2H4+C4H7Or_Olef_5 5.05E13 0.000 28632.2
C6H10_Olef_6+H=C6H11r_Olef_21.64E14 0.000 5377.5
DUP
OH+C6H10_Olef_6=H2O+C*CCJC*CC 1.56E6 2.300 -1362.3
HO2+C6H8O_Olef_9=H2O2+C6H7Or_Olef 1.18E-4 4.900 3680.6
C5H9r_Olef_2=C2H2+NC3H7 5.18E14 0.000 34105.3
C*CCJCCC=C6H11r_Olef_4 6.87E9 0.000 29205.8
CH2OH+C6H10_Olef_3=CH3OH+C6H9-A 5.66E12 0.000 18331.3
CH2OH+C6H10_Olef_1=CH3OH+C*CCJC*CC 1.22E13 0.000 16658.3
C3H5Or_Olef_1+C6H10=C3H5OH+C6H9-A 3.11E13 0.000 12165.1
C6H11O3r_5=C6H11O3r_7 2.91E12 -0.230 22298.7
C6H11Or_Olef_49=C3H6+C3H5Or_Olef_1 9.15E12 0.000 20554.0
C6H11Or_Olef_39=C6H10_Olef_1+OH 3.00E13 0.000 26799.1
C4H71-3+C6H10_Olef_1=C4H8-1+C6H9r_Olef 3.35E13 0.000 31356.8
C5H7Or_Olef=>C4H71-4+CO 3.30E12 0.620 17298.8
C6H9O4r_Olef_13=C6H8O3_Olef_4+OH 4.66E7 1.400 28658.5
C6H10_Olef_3+H=C6H11 6.75E13 0.000 4803.9
O2+C6H9-A=C6H9O2r_Olef 2.90E7 1.590 1080.3
DUP
C4H5-N+C6H10_Olef_1=C4H6+C6H9r_Olef 3.01E13 0.000 12882.1
C4H71-1+C6H10_Olef_1=C4H8-1+C6H9r_Olef 3.01E13 0.000 12882.1

O2+C*CCJC*CC=C6H9O2r_Olef_4 2.90E7 1.590 1080.3
DUP
H+C5H6O_Olef_1=H2+C*CC*CCJ*O7.15E5 2.400 1577.4
C2H3+C6H10_Olef_6=C2H4+C*CCJC*CC 1.49E13 0.000 9034.2
O2+CPC*CCJC*C=C6H9O4r_Olef_17 2.90E7 1.590 1080.3
DUP
HO2+C6H10_Olef_3=H2O2+C*CCJC*CC 5.12E-2 4.400 13546.5
C3H5Or_Olef+C6H10_Olef_3=IC3H5OH+C6H9-A 1.66E13 0.000 26098.8
C6H9O2r_Olef_15=C6H9O2r_Olef_16 9.82E0 2.655 18214.2
C*CCJC*CC+HO2=C6H10O2_Olef_83.35E10 0.600 -2105.6
DUP
CPC*CCJC*C=C6H8O_Olef_2+OH 3.50E10 0.100 9330.6
C3H5Or_Olef_1+C6H10_Olef_3=C3H5OH+C*CCJC*CC 1.78E13 0.000 9918.5
C6H9-A+HO2=C6H10O2_Olef_10 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_34=C6H11Or_Olef_39 6.00E11 0.000 33531.7
C6H11Or_Olef_26=C3H6+C3H5Or_Olef 9.15E12 0.000 20554.0
HO2+C6H10_Olef_1=H2O2+C*CCJC*CC 5.12E-2 4.400 13546.5
C3H5Or_Olef_1+C6H10_Olef_3=SC3H5OH+C*CCJC*CC 1.92E13 0.000 22179.2
O2+CPC*CCJC*C=C6H9O4r_Olef_17 2.90E7 1.590 1080.3
DUP
C*CCCCJ=C*CCJCCC 6.00E11 0.000 20052.1
PC2H4OH+C6H10_Olef_3=C2H5OH+C*CCJC*CC 2.89E12 0.000 11209.1
O2+CPC*CCJC*C=C6H9O4r_Olef_17 2.90E7 1.590 1080.3
DUP
CH3+C6H10_Olef_1=CH4+C6H9r_Olef 3.10E13 0.000 17686.0
C6H10_Olef_3+H=C6H11r_Olef_25.56E13 0.000 3847.9
DUP
CH2OH+C6H10_Olef_6=CH3OH+C*CCJC*CC 1.13E13 0.000 18331.3
C4H71-1+C6H10_Olef_1=C4H8-1+C*CCJC*CC 1.61E13 0.000 7361.2
C6H10O2_Olef_10=>C6H9Or_Olef_12+OH 1.59E20 -1.500 42857.5
CH3+C*CC*CC=CH4+C*CC*CCJ 7.68E12 0.000 13838.1
CH3+C6H10_Olef_3=CH4+C6H9-A 7.68E12 0.000 13838.1
C6H11Or_Olef_4=C3H5-A+IC3H5OH 5.46E13 0.000 21103.7
SC2H4OH+C6H10_Olef_1=C2H5OH+C*CCJC*CC 2.33E13 0.000 16849.5
O2+C*cy(CC*CCC)=HO2+C*cy(CCJC*CC) 2.00E13 0.000 29334.1
SC2H4OH+C6H10_Olef_3=C2H5OH+C6H9-A 1.08E13 0.000 18522.5
!C*CCCCJCOH=C3H5-A+C3H5OH 9.15E12 0.000 20554.0
C3H5-A+C3H5OH=C*CCCCJCOH 3.12E+03 2.53 11000 ! RDB - changed to
Kun x2
C4H71-4+C*CCC*C=C4H8-1+C*CC*CCJ 2.89E12 0.000 11209.1
CH3+C6H10O_Olef_11=CH4+C6H9Or_Olef_5 5.00E0 3.600 4328.3
O2+CPC*CCJC*C=C6H9O4r_Olef_10 2.90E7 1.590 1080.3
DUP
C6H11Or_Olef_27=C2H4+C4H7Or_Olef_1 5.05E13 0.000 28632.2
C6H9Or_Olef_5=C2H5+C4H4O_Olef 1.72E14 0.000 37379.6
H+C6H8O_Olef_15=H2+C6H7Or_Olef_1 7.15E5 2.400 1577.4
C6H10_Olef_1+H=C6H11r_Olef_77.85E13 0.000 5951.1
DUP
C4H71-1+C*CC*CC=C4H8-1+C*CC*CCJ 7.46E12 0.000 9034.2
cy(C*CC*CCC)+H=cy(C*CCJCCC) 1.22E14 0.000 3704.5
C*CCJCCC=C6H11r_Olef_1 3.00E11 0.000 31691.4
!O2+C*CCCCJCOH=C6H11O3r_5 3.02E15 -0.920 -129.1
!DUP
C4H71-3+C6H10_Olef_1=C4H8-2+C*CCJC*CC 1.79E13 0.000 24425.8
C6H11Or_Olef_23=C6H11Or_Olef_27 9.00E11 0.000 37953.2
O2+CPC*CCJC*C=C6H9O4r_Olef_10 2.90E7 1.590 1080.3
DUP

NC3H7+C6H10_olef_3=C3H8+C*CCJC*CC 1.92E12 0.000 10539.9
 CH2OH+C6H10_olef_1=CH3OH+C6H9r_olef 2.15E13 0.000 22179.2
 C*CCJC*CC+HO2=C6H10O2_olef_83.35E10 0.600 -2105.6
 DUP
 C*cy(CC*CCC)+H=C6H9r_R5_9 6.11E13 0.000 3704.5
 C6H11Or_olef_31=C6H10_olef_3+OH 3.00E13 0.000 26799.1
 O2+Ccy(C*CCC*C)=HO2+Ccy(CJC*CC*C) 2.00E13 0.000 32514.3
 C6H11Or_olef_23=C2H5+C4H6O_olef 1.72E14 0.000 37379.6
 C6H11r_olef_4=C2H4+C4H71-3 1.51E13 0.000 20745.2
 C6H11Or_olef_1=C6H11Or_olef_3 6.00E11 0.000 20721.3
 C3H5Or_olef_1+C6H10=SC3H5OH+C6H9-A 3.58E13 0.000 24425.8
 C3H5-A+C6H10_olef_6=C3H6+C*CCJC*CC 3.32E13 0.000 26098.8
 C*CCJC*CC+HO2=C6H10O2_olef_15 3.35E10 0.600 -2105.6
 DUP
 C3H5Or_olef+C6H10_olef_6=IC3H5OH+C*CCJC*CC 3.32E13 0.000 26098.8
 CH3+C6H10=CH4+C6H9-A 3.31E13 0.000 12165.1
 OH+C*CC*CC=H2O+C*CC*CCJ 7.80E5 2.300 -1362.3
 C*cy(CCC*CC)+H=C6H9r_R5_2 1.26E14 0.000 3250.4
 C*CCJCCC=C6H11 4.80E12 0.000 52484.4
 C4H71-3+C6H10=C4H8-2+C6H9-A 3.58E13 0.000 24425.8
 CH3+C6H8O_olef_15=CH4+C6H7Or_olef_1 5.00E0 3.600 4328.3
 C6H11Or_olef_7=C3H5-S+IC3H5OH 2.51E14 0.000 36901.6
 C6H11Or_olef_33=C6H11Or_olef_55 4.80E12 0.000 43498.0
 C2H3+C6H10_olef_1=C2H4+C*CCJC*CC 1.61E13 0.000 7361.2
 C4H71-3+C6H10_olef_1=C4H8-2+C6H9r_olef 2.72E13 0.000 29946.7
 C2H5+C6H10_olef_3=C2H6+C*CCJC*CC 2.89E12 0.000 11209.1
 C4H71-3+C*CC*CC=C4H8-2+C*CC*CCJ 8.29E12 0.000 26098.8
 CH3+C6H10_olef_6=CH4+C*CCJC*CC 1.54E13 0.000 13838.1
 C4H71-1+C6H10_olef_6=C4H8-1+C*CCJC*CC 1.49E13 0.000 9034.2
 C3H5-S+C6H10=C3H6+C6H9-A 3.22E13 0.000 7361.2
 NC3H7+C6H10_olef_6=C3H8+C*CCJC*CC 1.65E12 0.000 14459.5
 HO2+C*CCCC*O=H2O2+C6H9Or_olef_6 1.18E-4 4.900 3680.6
 C6H10_olef_3+H=C6H11r_olef_46.46E13 0.000 5377.5
 DUP
 C4H71-3+C*CC*CC=C4H8-1+C*CC*CCJ 1.07E13 0.000 27508.9
 PC2H4OH+C6H10_olef_1=C2H5OH+C*CCJC*CC 2.69E12 0.000 13455.7
 C3H5-A+C6H10_olef_3=C3H6+C*CCJC*CC 3.85E13 0.000 22179.2
 C6H9-A+HO2=C6H10O2_olef_10 3.35E10 0.600 -2105.6
 DUP
 Ccy(C*CC*CC)+H=C6H9r_R5 8.20E13 0.000 5377.5
 C6H9O2r_olef_16=C*CC*CC*C+HO2 1.83E10 0.790 15099.6
 HO2+C6H10_olef_6=H2O2+C*CCJC*CC 1.54E-1 4.400 13546.5
 O2+C6H9O2r_olef_16=C6H9O4r_olef_7 2.90E7 1.590 1080.3
 DUP
 C2H3+C*CCC*C=C2H4+C*CC*CCJ 1.73E13 0.000 5114.6
 O2+CPC*CCJC*C=C6H9O4r_olef_10 2.90E7 1.590 1080.3
 DUP
 CPC*CCJC*C=C*CC*CC*C+HO2 1.83E10 0.790 15099.6
 C*cy(CC*CCC)+H=C6H9r_R5_7 8.20E13 0.000 5377.5
 CH2OH+C6H10=CH3OH+C6H9-A 2.44E13 0.000 16658.3
 CH3+C6H10_olef_1=CH4+C*CCJC*CC 1.66E13 0.000 12165.1
 H+C6H10O_olef_11=H2+C6H9Or_olef_5 7.15E5 2.400 1577.4
 HO2+C*CCC*C=H2O2+C*CC*CCJ 5.12E-2 4.400 13546.5
 C4H71-3+C6H10_olef_6=C4H8-2+C*CCJC*CC 1.66E13 0.000 26098.8
 C2H5+C6H10_olef_1=C2H6+C*CCJC*CC 2.69E12 0.000 13455.7
 PC2H4OH+C6H10_olef_6=C2H5OH+C*CCJC*CC 2.49E12 0.000 15128.7
 OH+C6H10O_olef_4=H2O+C6H9Or_olef 2.30E4 2.600 -2079.3
 C6H11O3r_1=C*CCCC*O+CH2O2H 3.00E13 0.220 14098.6

OH+C6H10O_olef_9=H2O+C6H9Or_olef_3	6.13E4	2.700	-4588.8
PC2H4OH+C6H10_olef_3=C2H5OH+C6H9-A	1.25E12	0.000	15128.7
C5H7Or_olef=C3H5-A+CH2CO	3.52E13	0.000	30711.5
C6H10_olef_6+H=C6H11r_olef_11	2.2E14	0.000	3704.5
C2H3+C6H10_olef_3=C2H4+C*CCJC*CC	1.73E13	0.000	5114.6
C6H10_olef_1+H=C6H11r_olef_7	7.85E13	0.000	5951.1
DUP			
C3H5-S+C6H10_olef_1=C3H6+C*CCJC*CC	1.61E13	0.000	7361.2
Ccy(C*CCC*C)+H=C6H9r_R5_5	2.64E13	0.000	6166.2
OH+C6H10O_olef_6=H2O+C6H9Or_olef_2	6.13E4	2.700	-4588.8
CH3+C5H6O_olef_1=CH4+C*CC*CCJ*O	5.00E0	3.600	4328.3
CH3+C6H10O_olef_9=CH4+C6H9Or_olef_3	5.00E0	3.600	4328.3
H+C6H10_olef_3=H2+C*CCJC*CC	2.01E14	0.000	6190.1
C6H10_olef_3+H=C6H11r_olef_4	6.46E13	0.000	5377.5
DUP			
C4H71-3+C6H10_olef_3=C4H8-1+C6H9-A	1.04E13	0.000	27508.9
C6H9Or_olef_2=C4H71-3+CH2CO	1.06E14	0.000	30711.5
O2+CPC*CCJC*C=C6H9O4r_olef_17	2.90E7	1.590	1080.3
DUP			
NC3H7+C*CCC*C=C3H8+C*CC*CCJ	1.92E12	0.000	10539.9
C*CC*CC*C+H=C*CCJC*CC	1.01E14	0.000	2748.5
C6H9Or_olef_6=C4H71-4+CH2CO	3.52E13	0.000	30711.5
C4H71-3+C6H10_olef_3=C4H8-2+C*CCJC*CC	1.92E13	0.000	22179.2
O2+C6H9-A=C6H9O2r_olef_15	2.90E7	1.590	1080.3
DUP			
!C3H5-A+C*CC*CC=C3H6+C*CC*CCJ	1.66E13	0.000	26098.8
OH+C*CC*COH=H2O+C*CCJC*COH	2.30E4	2.600	-2079.3
Ccy(CC*CC*C)+H=C6H9r_R5_5	1.64E14	0.000	5377.5
DUP			
C2H5+C6H10_olef_1=C2H6+C6H9r_olef_1	4.96E12	0.000	18976.6
C*CCCCJCP=C*CCCcy(COC)+OH	2.28E8	1.290	9889.8
C6H11r_olef_1=C*CC*CC+CH3	2.39E14	0.000	39458.9
C6H11Or_olef_33=C4H71-4+C2H3OH	1.98E14	0.000	29731.6
C6H9O2r_olef_16=C6H8O_olef_2+OH	3.50E10	0.100	9330.6
C6H11Or_olef_32=C4H6+PC2H4OH	1.72E14	0.000	37379.6
C*CCJC*CC+HO2=C6H10O2_olef_8	3.35E10	0.600	-2105.6
DUP			
C*CCJC*CC+HO2=C6H10O2_olef_15	3.35E10	0.600	-2105.6
DUP			
!O2+C6H10_olef_1=HO2+C*CCJC*CC	2.00E13	0.000	21119.2
C6H9-A+HO2=C6H10O2_olef_5	3.35E10	0.600	-2105.6
DUP			
NC3H7+C6H10_olef_1=C3H8+C*CCJC*CC	1.78E12	0.000	12786.5
!C6H11=C3H5-A+C3H6	9.15E12	0.000	20554.0
C3H5-A+C3H6=C6H11	1.56E+03	2.53	11000 ! RDB changed to Kun
C4H71-3+C6H10_olef_1=C4H8-1+C*CCJC*CC	2.31E13	0.000	25835.9
C4H5-N+C*CCC*C=C4H6+C*CC*CCJ	1.73E13	0.000	5114.6
Ccy(C*CCC*C)+H=C6H9r_R5_1	6.81E13	0.000	3250.4
C2H5+C*CC*CC=C2H6+C*CC*CCJ	1.25E12	0.000	15128.7
C6H9-A+HO2=C6H10O2_olef_5	3.35E10	0.600	-2105.6
DUP			
C6H11Or_olef_34=C*CC*CC+CH2OH	3.72E14	0.000	35873.9
C6H10_olef_1+H=C*CCJCCC	6.11E13	0.000	3704.5
H+C6H8O_olef_9=H2+C6H7Or_olef_1	7.15E5	2.400	1577.4
C3H5Or_olef_1+C6H10_olef_3=C3H5OH+C6H9-A	6.96E12	0.000	13838.1
HO2+C6H8O_olef_15=H2O2+C6H7Or_olef_1	1.18E-4	4.900	3680.6
O2+CPC*CCJC*C=C6H9O4r_olef_13	2.90E7	1.590	1080.3
DUP			

PC2H4OH+C6H10_olef_1=C2H5OH+C6H9r_olef 5.03E12 0.000 18976.6
 C*CCJCCC=C4H6+C2H5 1.72E14 0.000 37379.6
 C3H5Or_olef_1+C6H10_olef_3=SC3H5OH+C6H9-A 8.14E12 0.000 26098.8
 C*CCJC*CC+HO2=C6H10O2_olef_15 3.35E10 0.600 -2105.6
 DUP
 H+C*CCC*C=H2+C*CC*CCJ 2.01E14 0.000 6190.1
 C2H3+C6H10_olef_3=C2H4+C6H9-A 7.46E12 0.000 9034.2
 !O2+C6H11Or_olef_1=C6H11O3r_3 5.20E11 0.230 -1579.8 ! Disabled
 Waddington
 !DUP
 C4H71-4+C6H10_olef_1=C4H8-1+C6H9r_olef 5.01E12 0.000 18976.6
 C4H71-4+C6H10=C4H8-1+C6H9-A 5.38E12 0.000 13455.7
 C*CCJC*CC+HO2=C6H10O2_olef_23.35E10 0.600 -2105.6
 DUP
 C4H71-3+C*CCC*C=C4H8-2+C*CC*CCJ 1.92E13 0.000 22179.2
 O2+C*CCJC*CC=C6H9O2r_olef_6 2.90E7 1.590 1080.3
 DUP
 Ccy(C*CCC*C)+H=C6H9r_R5_10 6.11E13 0.000 3704.5
 C4H71-4+C6H10_olef_3=C4H8-1+C6H9-A 1.25E12 0.000 15128.7
 C4H71-4+C*CC*CC=C4H8-1+C*CC*CCJ 1.25E12 0.000 15128.7
 CH3+cy(C*CCCC)=CH4+cy(C*CCJCCC) 2.47E13 0.000
 10946.2
 C2H3+cy(C*CCC*CC)=C2H4+cy(C*CC*CCJC) 3.41E13 0.000
 15367.7
 HO2+cy(C*CCC*CC)=H2O2+cy(C*CC*CCJC) 1.02E-1 4.400
 13546.5
 CH3+cy(C*CCCC)=CH4+cy(C*CCCJCC) 2.68E13 0.000
 19741.4
 C2H5+cy(C*CCCC)=C2H6+cy(C*CCCJCC) 4.34E12 0.000
 21032.0
 H+cy(C*CCCC)=H2+cy(C*CCJCCC) 2.60E14 0.000
 7074.4
 HO2+cy(C*CC*CCC)=H2O2+cy(C*CC*CCJC) 1.02E-1 4.400
 13546.5
 HO2+cy(C*CCCC)=H2O2+cy(C*CCJCCC) 1.02E-1 4.400
 13546.5
 C2H5+cy(C*CCCC)=C2H6+cy(C*CCJCCC) 4.00E12 0.000
 12236.8
 cy(C*CCCC)+H=cy(CJCCCC) 1.35E14 0.000 4803.9
 OH+cy(C*CC*CCC)=H2O+cy(C*CC*CCJC) 0.52E6 2.300 -
 1362.3 ! /2 RDB
 C3H5-A+cy(C*CCCC)=C3H6+cy(C*CCCJCC) 4.90E13 0.000
 32002.1
 H+cy(C*CCCC)=H2+cy(C*CCCJCC) 3.98E14 0.000
 9846.8
 C2H3+cy(C*CCCC)=C2H4+cy(C*CCCJCC) 2.60E13 0.000
 14937.5
 C2H5+cy(C*CC*CCC)=C2H6+cy(C*CC*CCJC) 5.69E12 0.000
 21462.2
 C2H5+cy(C*CCC*CC)=C2H6+cy(C*CC*CCJC) 5.69E12 0.000
 21462.2
 OH+cy(C*CCC*CC)=H2O+cy(C*CC*CCJC) 0.52E6 2.300 -
 1362.3 ! /2 RDB
 C3H5-A+cy(C*CCCC)=C3H6+cy(C*CCJCCC) 5.33E13 0.000
 23206.9
 OH+cy(C*CCCC)=H2O+cy(C*CCJCCC) 1.04E6 2.300 -
 1362.3

C2H3+cy (C*CC*CCC) =C2H4+cy (C*CC*CCJC) 15367.7	3.41E13	0.000	
C2H3+cy (C*CCCC) =C2H4+cy (C*CCJCCC) 6142.3	2.40E13	0.000	
C2H3+Ccy (C*CCC*C) =C2H4+Ccy (CJC*CC*C) 15367.7	1.70E13	0.000	
OH+Ccy (C*CCC*C) =H2O+C*cy (CCJCC*C) 1362.3	7.80E5	2.300	-
C2H3+C*cy (CC*CCC) =C2H4+C*cy (CCJCC*C) 15367.7	1.70E13	0.000	
!H+Ccy (C*CCC*C) =H2+Ccy (CJC*CC*C) 6190.1	2.01E14	0.000	
OH+C*cy (CC*CCC) =H2O+C*cy (CCJCC*C) 1362.3	5.20E5	2.300	-
!H+Ccy (C*CC*CC) =H2+Ccy (CJC*CC*C) 6190.1	2.01E14	0.000	
HO2+Ccy (C*CCC*C) =H2O2+Ccy (CJC*CC*C) 13546.5	5.12E-2	4.400	
H+C*cy (CC*CCC) =H2+C*cy (CCJCC*C) 7074.4	1.30E14	0.000	
!CH3+Ccy (C*CC*CC) =CH4+C*cy (CCJC*CC) 13838.1	7.68E12	0.000	
C2H3+Ccy (CC*CC*C) =C2H4+Ccy (CJC*CC*C) 15367.7	8.52E12	0.000	
HO2+Ccy (CC*CC*C) =H2O2+Ccy (CJC*CC*C) 13546.5	2.56E-2	4.400	
C3H5-A+Ccy (C*CC*CC) =C3H6+C*cy (CCJC*CC) 26098.8	1.66E13	0.000	
!CH3+Ccy (C*CCC*C) =CH4+C*cy (CCJCC*C) 13838.1	7.68E12	0.000	
C2H5+Ccy (CC*CC*C) =C2H6+CJcy (CC*CC*C) 18976.6	4.99E12	0.000	
C2H5+Ccy (CC*CC*C) =C2H6+Ccy (CJC*CC*C) 21462.2	1.42E12	0.000	
OH+Ccy (C*CCC*C) =H2O+Ccy (CJC*CC*C) 1362.3	5.20E5	2.300	-
!H+Ccy (C*CCC*C) =H2+C*cy (CCJCC*C) 9177.6	7.28E13	0.000	
CH3+C*cy (CCC*CC) =CH4+C*cy (CCJC*CC) 20171.6	3.51E13	0.000	
H+C*cy (CC*CCC) =H2+C*cy (CCJC*CC) 7074.4	1.30E14	0.000	
OH+Ccy (C*CC*CC) =H2O+Ccy (CJC*CC*C) 1362.3	5.20E5	2.300	-
!CH3+Ccy (CC*CC*C) =CH4+Ccy (CJC*CC*C) 20171.6	8.78E12	0.000	
OH+Ccy (CC*CC*C) =H2O+Ccy (CJC*CC*C) 1362.3	2.60E5	2.300	-
!CH3+Ccy (C*CCC*C) =CH4+Ccy (CJC*CC*C) 20171.6	1.76E13	0.000	
!CH3+Ccy (C*CC*CC) =CH4+Ccy (CJC*CC*C) 20171.6	1.76E13	0.000	
C3H5-A+C*cy (CC*CCC) =C3H6+C*cy (CCJC*CC) 32432.3	3.79E13	0.000	
C3H5-A+Ccy (C*CCC*C) =C3H6+C*cy (CCJCC*C) 26098.8	1.66E13	0.000	
C2H3+Ccy (C*CC*CC) =C2H4+C*cy (CCJC*CC) 9034.2	7.46E12	0.000	

H02+C*cy (CCC*CC) =H2O2+C*cy (CCJC*CC) 13546.5	1.02E-1	4.400	
C3H5-A+Ccy (CC*CC*C) =C3H6+Ccy (CJC*CC*C) 32432.3	1.89E13	0.000	
C2H5+Ccy (C*CC*CC) =C2H6+C*cy (CCJC*CC) 15128.7	1.25E12	0.000	
C2H3+Ccy (CC*CC*C) =C2H4+CJcy (CC*CC*C) 12882.1	3.01E13	0.000	
C2H3+C*cy (CCC*CC) =C2H4+C*cy (CCJC*CC) 15367.7	3.41E13	0.000	
C3H5-A+Ccy (CC*CC*C) =C3H6+CJcy (CC*CC*C) 29946.7	5.54E13	0.000	
OH+C*cy (CC*CCC) =H2O+C*cy (CCJC*CC) 1362.3	5.20E5	2.300	-
!H+Ccy (CC*CC*C) =H2+CJcy (CC*CC*C) 12595.3	3.36E14	0.000	
!H+Ccy (CC*CC*C) =H2+Ccy (CJC*CC*C) 5401.4	5.38E13	0.000	
H02+C*cy (CC*CCC) =H2O2+C*cy (CCJC*CC) 13546.5	5.12E-2	4.400	
C2H5+C*cy (CCC*CC) =C2H6+C*cy (CCJC*CC) 21462.2	5.69E12	0.000	
H02+C*cy (CC*CCC) =H2O2+C*cy (CCJCC*C) 13546.5	5.12E-2	4.400	
C3H5-A+Ccy (C*CCC*C) =C3H6+Ccy (CJC*CC*C) 32432.3	3.79E13	0.000	
C2H3+Ccy (C*CCC*C) =C2H4+C*cy (CCJCC*C) 9034.2	7.46E12	0.000	
OH+Ccy (C*CC*CC) =H2O+C*cy (CCJC*CC) 1362.3	7.80E5	2.300	-
C2H5+Ccy (C*CCC*C) =C2H6+C*cy (CCJCC*C) 15128.7	1.25E12	0.000	
C2H5+Ccy (C*CC*CC) =C2H6+Ccy (CJC*CC*C) 21462.2	2.85E12	0.000	
C2H5+C*cy (CC*CCC) =C2H6+C*cy (CCJC*CC) 21462.2	2.85E12	0.000	
C3H5-A+C*cy (CC*CCC) =C3H6+C*cy (CCJCC*C) 32432.3	3.79E13	0.000	
C2H3+Ccy (C*CC*CC) =C2H4+Ccy (CJC*CC*C) 15367.7	1.70E13	0.000	
C3H5-A+C*cy (CCC*CC) =C3H6+C*cy (CCJC*CC) 32432.3	7.58E13	0.000	
H+C*cy (CCC*CC) =H2+C*cy (CCJC*CC) 6190.1	4.03E14	0.000	
CH3+C*cy (CC*CCC) =CH4+C*cy (CCJCC*C) 20171.6	1.76E13	0.000	
H02+Ccy (C*CC*CC) =H2O2+Ccy (CJC*CC*C) 13546.5	5.12E-2	4.400	
H02+Ccy (C*CC*CC) =H2O2+C*cy (CCJC*CC) 13546.5	7.68E-2	4.400	
C2H3+C*cy (CC*CCC) =C2H4+C*cy (CCJC*CC) 15367.7	1.70E13	0.000	
CH3+C*cy (CC*CCC) =CH4+C*cy (CCJC*CC) 20171.6	1.76E13	0.000	
!H+Ccy (C*CC*CC) =H2+C*cy (CCJC*CC) 9177.6	7.28E13	0.000	
OH+C*cy (CCC*CC) =H2O+C*cy (CCJC*CC) 1362.3	1.04E6	2.300	-

C3H5-A+Ccy (C*CC*CC) =C3H6+Ccy (CJC*CC*C) 32432.3		3.79E13	0.000	
H02+Ccy (C*CCC*C) =H2O2+C*cy (CCJCC*C) 13546.5		7.68E-2	4.400	
C2H5+Ccy (C*CCC*C) =C2H6+Ccy (CJC*CC*C) 21462.2		2.85E12	0.000	
!CH3+Ccy (CC*CC*C) =CH4+CJcy (CC*CC*C) 17686.0		3.10E13	0.000	
C2H5+C*cy (CC*CCC) =C2H6+C*cy (CCJCC*C) 21462.2		2.85E12	0.000	
C5H5+C6H10=C5H6+C6H9-A	7.04E14	0.000	33555.6	
C5H5+C4H6=C5H6+C4H5-N	3.98E14	0.000	41562.1	
C5H5+C4H6=C5H6+C4H5-I	4.51E14	0.000	39315.5	
CJcy (CCCC) =Ccy (CCJCCC)	4.80E12	0.000	38240.0	
C6H10+C3H5-A=C*CCCC (CJ) CC*C	1.10E12	0.000	18355.2	
DUP				
C6H10+C3H5-A=C*CCCC (CJ) CC*C	1.10E12	0.000	18355.2	
DUP				
C*CCCC (CJ) CC*C=C4H71-4+C*CCC*C	5.52E13	0.000	28536.6	
C6H10+C3H5-A=C*CCCCJCCC*C	2.23E12	0.000	16514.9	
C*CCCCJCC=C3H5-A+C4H8-1	9.15E12	0.000	20554.0	
C*CCCC (C) CJ=C4H71-4+C3H6	5.52E13	0.000	28536.6	
C6H10+CH3=C*CCCCJCC	1.10E12	0.000	9966.3	! RDB x3
C6H10+CH3=C*CCCC (C) CJ	5.40E12	0.000	11806.6	! RDB x3
DUP				
C6H10+CH3=C*CCCC (C) CJ	5.40E12	0.000	11806.6	! RDB x3
DUP				
!C*CCCC (C) CJ=C4H71-4+C3H6	5.52E13	0.000	28536.6	
!C*CCCC (C) CJ=C6H10+CH3	7.68E13	0.000	30615.9	
!C*CCCCJCC=C3H5-A+C4H8-1	9.15E12	0.000	20554.0	
!C*CCCCJCC=C6H10+CH3	4.27E13	0.000	30520.3	
C*CC*CC+H=CC*CCCJ	7.85E13	0.000	5951.1	
DUP				
C*CC*CC+H=CC*CCJC	5.03E13	0.000	2748.5	
C*CC*CC+H=CC*CCCJ	7.85E13	0.000	5951.1	
DUP				
C3H6+C2H3=C*CCCJC	1.37E12	0.000	6309.6	
C*CCCC (CJ) CC*C=C*CCJCC (C) CC*C	6.00E11	0.000	19765.3	
C*CCJCC (C) CC*C=C4H6+C*CCCJC	2.14E14	0.000	35085.2	
H+C*CCCC=H2+C*CCCJC	1.99E14	0.000	9846.8	
H+CC*CCC=H2+CC*CCJC	1.59E14	0.000	7361.2	
CH3+C*CCCC=CH4+C*CCCJC	2.22E13	0.000	15391.6	
H+CC*CCC=H2+C*CCJCC	7.28E13	0.000	9177.6	
H+cy (C*CCCC) =H2+C5H7	2.60E14	0.000	7074.4	
CH3+C*CCCC=CH4+C*CCCCJ	2.36E13	0.000	17255.8	
H+cy (C*CCCC) =H2+cy (C*CCCJC)	1.99E14	0.000	9846.8	
H02+CC*CCC=H2O2+C*CCJCC	7.68E-2	4.400	13546.5	
H+C*CCCC=H2+C*CCJCC	1.30E14	0.000	7074.4	
OH+CC*CCC=H2O+C*CCJCC	7.80E5	2.300	-1362.3	
CH3+CC*CCC=CH4+CC*CCCJ	3.10E13	0.000	17686.0	
H02+cy (C*CCCC) =H2O2+C5H7	1.02E-1	4.400	13546.5	
OH+C*CCCC=H2O+C*CCJCC	5.20E5	2.300	-1362.3	
H+CC*CCC=H2+CC*CCCJ	2.87E14	0.000	12499.7	
CH3+CC*CCC=CH4+C*CCJCC	7.68E12	0.000	13838.1	
H02+CC*CCC=H2O2+CC*CCJC	5.12E-2	4.400	13546.5	
CH3+CC*CCC=CH4+CC*CCJC	1.66E13	0.000	12165.1	
OH+CC*CCC=H2O+CC*CCJC	5.20E5	2.300	-1362.3	
OH+cy (C*CCCC) =H2O+C5H7	1.04E6	2.300	-1362.3	

H+C*CCCC=H2+C*CCCCJ	2.87E14	0.000	12499.7	
CH3+C*CCCC=CH4+C*CCJCC	1.26E13	0.000	11734.9	
HO2+C*CCCC=H2O2+C*CCJCC	5.12E-2	4.400	13546.5	
CH3+cy (C*CCCC) =CH4+cy (C*CCCJC)	1.76E13	0.000	20171.6	
C*CCCC (CJ) CC=C4H71-4+C4H8-1	5.52E13	0.000	28536.6	
C*CC (CJ) CCC*C=C4H71-4+C4H6	3.06E13	0.000	25238.4	
C*CCCC (CJ) CC=C*CCJCC (C) CC	6.00E11	0.000	19765.3	
C*CCCCJCCC=C3H5-A+C*CCCC	9.15E12	0.000	20554.0	
C*CC (CJ) CCC*C=C*CC (C) CCJC*C	6.00E11	0.000	20721.3	
C*CC (C) CCJC*C=C4H6+C4H71-3	4.19E13	0.000	28058.6	
C6H10+C2H3=C*CCCJCCC*C	2.74E12	0.000	6309.6	
C6H10+C2H5=C*CCCC (CJ) CC	1.88E11	0.000	11304.7	
DUP				
C*CCJCC (C) CC=C4H6+SC4H9	2.14E14	0.000	35085.2	
C6H10+C2H5=C*CCCCJCCC	3.83E11	0.000	9464.4	
C*CCCC (C) CJ=C*CCJCC (C) C	6.00E11	0.000	19765.3	
C6H10+C2H3=C*CC (CJ) CCC*C	1.35E12	0.000	8149.9	
DUP				
C6H10+C2H5=C*CCCC (CJ) CC	1.88E11	0.000	11304.7	
DUP				
C6H10+C2H3=C*CC (CJ) CCC*C	1.35E12	0.000	8149.9	
DUP				
C*CCJCC (C) C=C4H6+IC3H7	2.14E14	0.000	35085.2	
C*CCCJCCC*C=C*CCC*C+C3H5-A	9.15E12	0.000	20554.0	
C3H5-A+C6H10=C3H6+CJ*CCCC*C	3.78E13	0.000	32432.3	
C3H5-S+C6H10=C3H6+C*CJCCC*C	2.56E13	0.000	13168.9	
C3H5-T+C6H10=C3H6+C*CJCCC*C	1.88E13	0.000	14172.7	
CJ*CCCC*C=C*CJCCC*C	1.85E10	0.000	13862.0	
C2H5+C6H10=C2H6+CJ*CCCC*C	3.31E12	0.000	21462.2	
CJ*CCCC*C=C2H2+C4H71-4	5.18E14	0.000	34105.3	
C3H3+C6H10=C3H4-A+C*CJCCC*C	1.18E13	0.000	26552.9	
C*CJCCC*C=C3H5-A+C3H4-A	9.00E+10	1.02	28400	! -3kcal
RDB original Genesys	6.55E13	0.000	23541.5	
C2H3+C6H10=C2H4+C*CJCCC*C	2.56E13	0.000	13168.9	
C3H5-T+C6H10=C3H6+CJ*CCCC*C	1.62E13	0.000	16371.5	
H+C6H10=H2+C*CJCCC*C	2.93E14	0.000	14053.2	
C2H3+C6H10=C2H4+CJ*CCCC*C	2.28E13	0.000	15367.7	
C3H5-A+C6H10=C3H6+C*CJCCC*C	4.21E13	0.000	30233.5	
CH3+C6H10=CH4+CJ*CCCC*C	2.18E13	0.000	20171.6	
C3H3+C6H10=C3H4-A+CJ*CCCC*C	1.00E13	0.000	28751.7	
H+C6H10=H2+CJ*CCCC*C	3.61E14	0.000	17231.9	
C3H3+C6H10=C3H4-P+CJ*CCCC*C	1.01E13	0.000	28751.7	
C3H5-S+C6H10=C3H6+CJ*CCCC*C	2.30E13	0.000	15367.7	
CJ*CCCC*C=C6H9-A	3.00E11	0.000	15057.0	
DUP				
C2H5+C6H10=C2H6+C*CJCCC*C	3.87E12	0.000	19263.4	
CJ*CCCC*C=C6H9-A	2.40E12	0.000	31452.4	
DUP				
C3H3+C6H10=C3H4-P+C*CJCCC*C	1.19E13	0.000	26552.9	
CH3+C6H10=CH4+C*CJCCC*C	2.54E13	0.000	17972.8	
C*CJCCC*C=C6H9-A	2.40E12	0.000	31787.0	
C2H4O3=>OH+C (*O) COJ	1.59E20	-1.500	42857.5	
C (*O) COJ=CH2O+HCO	3.00E13	0.220	14098.6	
C2H3+C*Ccy (CCC*CC) =C2H4+C7H9r_R5_17	8.52E12	0.000	15367.7	
C2H3+C*Ccy (CCC*CC) =C2H4+C7H9r_R5_18	3.41E13	0.000	15367.7	
C2H3+Ccy (C*CC*C (C) C) =C2H4+C7H9r_Olef_4	1.70E13	0.000	15367.7	
C2H3+Ccy (C*CC*C (C) C) =C2H4+C7H9r_R5_22	1.49E13	0.000	9034.2	
C2H3+Ccy (C*CCC*C (C)) =C2H4+C7H9r_Olef_12	1.70E13	0.000	15367.7	

C2H3+Ccy(C*CCC*(C))=C2H4+C7H9r_R5_8	1.49E13	0.000	9034.2
C2H3+CCcyCC*CC*C=C2H4+CJCcyCC*CC*C	2.29E13	0.000	12451.9
C2H3+CCcyCC*CC*C=C2H4+CCJcyCC*CC*C	2.15E13	0.000	10587.7
C2H3+CCcyCC*CC*C=C2H4+CCcyCJC*CC*C	6.49E12	0.000	14937.5
C2H3+Ccy(C*CC(C)*CC)=C2H4+C7H9r_Olef_4	1.70E13	0.000	15367.7
C2H3+Ccy(C*CC(C)*CC)=C2H4+C7H9r_Olef_5	7.46E12	0.000	9034.2
C2H3+Ccy(C*CC(C)*CC)=C2H4+C7H9r_Olef_6	7.46E12	0.000	9034.2
C2H3+Ccy(CC*(C)(C)*C)=C2H4+C7H9r_Olef_2	7.46E12	0.000	9034.2
C2H3+Ccy(CC*(C)(C)*C)=C2H4+C7H9r_Olef_3	3.01E13	0.000	12882.1
C2H3+Ccy(CC*(C)(C)*C)=C2H4+C7H9r_Olef_4	8.52E12	0.000	15367.7
C2H3+CCcyC*CC*CC=C2H4+CJCcyC*CC*CC	3.01E13	0.000	12882.1
C2H3+CCcyC*CC*CC=C2H4+CCcyCJC*CC*C	1.70E13	0.000	15367.7
C2H3+CCcyC*CC*CC=C2H4+CC*cy(CCJC*CC)	1.61E13	0.000	7361.2
C2H3+CCcyC*CCC*C=C2H4+CJCcyC*CCC*C	3.01E13	0.000	12882.1
C2H3+CCcyC*CCC*C=C2H4+CC*cy(CCJCC*C)	1.61E13	0.000	7361.2
C2H3+CCcyC*CCC*C=C2H4+CCcyCJC*CC*C	1.70E13	0.000	15367.7
C2H3+Ccy(C*(C)(C)*CC)=C2H4+C7H9r_Olef_12	1.70E13	0.000	15367.7
C2H3+Ccy(C*(C)(C)*CC)=C2H4+C7H9r_R5_15	7.46E12	0.000	9034.2
C2H3+Ccy(C*(C)(C)*CC)=C2H4+C7H9r_R5_2	7.46E12	0.000	9034.2
C2H3+Ccy(CC(C)*CC*C)=C2H4+C7H9r_Olef_16	3.01E13	0.000	12882.1
C2H3+Ccy(CC(C)*CC*C)=C2H4+C7H9r_Olef_12	8.52E12	0.000	15367.7
C2H3+Ccy(CC(C)*CC*C)=C2H4+C7H9r_R5_1	7.46E12	0.000	9034.2
C2H3+Ccy(CC*CC*CC)=C2H4+CJcy(CC*CC*CC)	3.01E13	0.000	12882.1
C2H3+C7H10_R5_10=C2H4+CC*cy(CCJC*CC)	1.70E13	0.000	15367.7
C2H3+C7H10_R5_10=C2H4+C7H9r_R5_17	7.46E12	0.000	9034.2
C2H3+C7H10_R5_11=C2H4+C7H9r_R5_18	1.30E13	0.000	14937.5
C2H3+C7H10_R5_11=C2H4+C7H9r_R5_21	1.70E13	0.000	15367.7
C2H3+C7H10_R5_11=C2H4+C7H9r_R5_5	6.49E12	0.000	14937.5
C2H3+C7H10_R5_13=C2H4+C7H9r_Olef_6	1.70E13	0.000	15367.7
C2H3+C7H10_R5_13=C2H4+C7H9r_R5_10	7.46E12	0.000	9034.2
C2H3+C7H10_R5_13=C2H4+C7H9r_R5_22	1.70E13	0.000	15367.7
C2H3+C7H10_R5_15=C2H4+C7H9r_R5_22	8.52E12	0.000	15367.7
C2H3+C7H10_R5_15=C2H4+C7H9r_R5_25	3.01E13	0.000	12882.1
C2H3+C7H10_R5_15=C2H4+C7H9r_Olef_2	1.70E13	0.000	15367.7
C2H3+C7H10_R5_1=C2H4+C7H9r_R5_3	2.78E12	0.000	9440.5
C2H3+C7H10_R5_1=C2H4+C7H9r_R5_4	4.24E12	0.000	9010.3
C2H3+C7H10_R5_2=C2H4+C7H9r_R5_5	1.30E13	0.000	14937.5
C2H3+C7H10_R5_2=C2H4+C*CCy(C*CCCJC)	1.70E13	0.000	15367.7
C2H3+C7H10_R5_2=C2H4+C7H9r_R5_7	1.30E13	0.000	14937.5
C2H3+C7H10_R5_3=C2H4+C7H9r_R5_2	1.70E13	0.000	15367.7
C2H3+C7H10_R5_3=C2H4+C7H9r_R5_4	7.46E12	0.000	9034.2
C2H3+C7H10_R5_3=C2H4+C7H9r_R5_8	1.70E13	0.000	15367.7
C2H3+C7H10_R5_4=C2H4+C7H9r_Olef_5	1.70E13	0.000	15367.7
C2H3+C7H10_R5_4=C2H4+C7H9r_Olef_6	1.70E13	0.000	15367.7
C2H3+C7H10_R5_4=C2H4+C7H9r_R5_9	7.46E12	0.000	9034.2
C2H3+C7H10_R5_5=C2H4+C7H9r_R5_10	5.56E12	0.000	9440.5
C2H3+C7H10_R5_5=C2H4+C7H9r_R5_9	2.78E12	0.000	9440.5
C2H3+C7H10_R5_6=C2H4+CC*cy(CCJCC*C)	1.70E13	0.000	15367.7
C2H3+C7H10_R5_6=C2H4+CC*cy(CCJC*CC)	1.70E13	0.000	15367.7
C2H3+C7H10_R5_6=C2H4+C7H9r_R5_5	7.46E12	0.000	9034.2
C2H3+C7H10_R5_8=C2H4+C7H9r_R5_12	3.01E13	0.000	12882.1
C2H3+C7H10_R5_8=C2H4+C7H9r_R5_1	1.70E13	0.000	15367.7
C2H3+C7H10_R5_8=C2H4+C7H9r_R5_2	8.52E12	0.000	15367.7
C2H3+C7H10_R5_9=C2H4+C7H9r_R5_1	1.70E13	0.000	15367.7
C2H3+C7H10_R5_9=C2H4+C7H9r_R5_15	8.52E12	0.000	15367.7
C2H3+C7H10_R5_9=C2H4+C7H9r_R5_16	3.01E13	0.000	12882.1
C2H3+C*CCCC*CC=C2H4+C*CCC*CCJC	1.61E13	0.000	7361.2
C2H3+C*CCCC*CC=C2H4+C*CCCCJC*C	7.46E12	0.000	9034.2

C2H3+C*CCCC*CC=C2H4+C*CCJCC*CC	1.61E13	0.000	7361.2
C2H3+C*CC(C)CC*C=C2H4+C7H11r_Olef	5.34E12	0.000	5903.3
C2H3+C*CC(C)CC*C=C2H4+C7H11r_Olef_23	3.01E13	0.000	12882.1
C2H3+C*CC(C)CC*C=C2H4+C7H11r_Olef_2	1.61E13	0.000	7361.2
C2H5+C*Ccy(CCC*CC)=C2H6+C7H9r_R5_17	1.42E12	0.000	21462.2
C2H5+C*Ccy(CCC*CC)=C2H6+C7H9r_R5_18	5.69E12	0.000	21462.2
C2H5+Ccy(C*CC*C(C)C)=C2H6+C7H9r_Olef_4	2.85E12	0.000	21462.2
C2H5+Ccy(C*CC*C(C)C)=C2H6+C7H9r_R5_22	2.49E12	0.000	15128.7
C2H5+Ccy(C*CCC*C(C))=C2H6+C7H9r_Olef_12	2.85E12	0.000	21462.2
C2H5+Ccy(C*CCC*C(C))=C2H6+C7H9r_R5_8	2.49E12	0.000	15128.7
C2H5+CCcyCC*CC*C=C2H6+CJCcyCC*CC*C	3.79E12	0.000	18546.4
C2H5+CCcyCC*CC*C=C2H6+CCJcyCC*CC*C	3.59E12	0.000	16682.2
C2H5+CCcyCC*CC*C=C2H6+CCcyCJC*CC*C	1.08E12	0.000	21032.0
C2H5+Ccy(C*CC(C)*CC)=C2H6+C7H9r_Olef_4	2.85E12	0.000	21462.2
C2H5+Ccy(C*CC(C)*CC)=C2H6+C7H9r_Olef_5	1.25E12	0.000	15128.7
C2H5+Ccy(C*CC(C)*CC)=C2H6+C7H9r_Olef_6	1.25E12	0.000	15128.7
C2H5+Ccy(CC*C(C)C*C)=C2H6+C7H9r_Olef_2	1.25E12	0.000	15128.7
C2H5+Ccy(CC*C(C)C*C)=C2H6+C7H9r_Olef_3	4.98E12	0.000	18976.6
C2H5+Ccy(CC*C(C)C*C)=C2H6+C7H9r_Olef_4	1.42E12	0.000	21462.2
C2H5+CCcyC*CC*CC=C2H6+CJCcyC*CC*CC	4.98E12	0.000	18976.6
C2H5+CCcyC*CC*CC=C2H6+CCcyCJC*CC*C	2.85E12	0.000	21462.2
C2H5+CCcyC*CC*CC=C2H6+CC*cy(CCJC*CC)	2.69E12	0.000	13455.7
C2H5+CCcyC*CCC*C=C2H6+CJCcyC*CCC*C	4.98E12	0.000	18976.6
C2H5+CCcyC*CCC*C=C2H6+CC*cy(CCJCC*C)	2.69E12	0.000	13455.7
C2H5+CCcyC*CCC*C=C2H6+CCcyCJC*CC*C	2.85E12	0.000	21462.2
C2H5+Ccy(C*C(C)C*CC)=C2H6+C7H9r_Olef_12	2.85E12	0.000	21462.2
C2H5+Ccy(C*C(C)C*CC)=C2H6+C7H9r_R5_15	1.25E12	0.000	15128.7
C2H5+Ccy(C*C(C)C*CC)=C2H6+C7H9r_R5_2	1.25E12	0.000	15128.7
C2H5+Ccy(CC(C)*CC*C)=C2H6+C7H9r_Olef_16	4.98E12	0.000	18976.6
C2H5+Ccy(CC(C)*CC*C)=C2H6+C7H9r_Olef_12	1.42E12	0.000	21462.2
C2H5+Ccy(CC(C)*CC*C)=C2H6+C7H9r_R5_1	1.25E12	0.000	15128.7
C2H5+Ccy(CC*CC*CC)=C2H6+CJcy(CC*CC*CC)	4.97E12	0.000	18976.6
C2H5+C7H10_R5_8=C2H6+C7H9r_R5_12	4.98E12	0.000	18976.6
C2H5+C7H10_R5_8=C2H6+C7H9r_R5_1	2.85E12	0.000	21462.2
C2H5+C7H10_R5_8=C2H6+C7H9r_R5_2	1.42E12	0.000	21462.2
C2H5+C7H10_R5_10=C2H6+CC*cy(CCJC*CC)	2.85E12	0.000	21462.2
C2H5+C7H10_R5_10=C2H6+C7H9r_R5_17	1.25E12	0.000	15128.7
C2H5+C7H10_R5_11=C2H6+C7H9r_R5_18	2.17E12	0.000	21032.0
C2H5+C7H10_R5_11=C2H6+C7H9r_R5_21	2.85E12	0.000	21462.2
C2H5+C7H10_R5_11=C2H6+C7H9r_R5_5	1.08E12	0.000	21032.0
C2H5+C7H10_R5_13=C2H6+C7H9r_Olef_6	2.85E12	0.000	21462.2
C2H5+C7H10_R5_13=C2H6+C7H9r_R5_10	1.25E12	0.000	15128.7
C2H5+C7H10_R5_13=C2H6+C7H9r_R5_22	2.85E12	0.000	21462.2
C2H5+C7H10_R5_15=C2H6+C7H9r_R5_22	1.42E12	0.000	21462.2
C2H5+C7H10_R5_15=C2H6+C7H9r_R5_25	4.97E12	0.000	18976.6
C2H5+C7H10_R5_15=C2H6+C7H9r_Olef_2	2.85E12	0.000	21462.2
C2H5+C7H10_R5_1=C2H6+C7H9r_R5_3	4.65E11	0.000	15535.0
C2H5+C7H10_R5_1=C2H6+C7H9r_R5_4	7.09E11	0.000	15104.8
C2H5+C7H10_R5_2=C2H6+C7H9r_R5_5	2.17E12	0.000	21032.0
C2H5+C7H10_R5_2=C2H6+C*Ccy(C*CCCJC)	2.85E12	0.000	21462.2
C2H5+C7H10_R5_2=C2H6+C7H9r_R5_7	2.17E12	0.000	21032.0
C2H5+C7H10_R5_3=C2H6+C7H9r_R5_2	2.85E12	0.000	21462.2
C2H5+C7H10_R5_3=C2H6+C7H9r_R5_4	1.25E12	0.000	15128.7
C2H5+C7H10_R5_3=C2H6+C7H9r_R5_8	2.85E12	0.000	21462.2
C2H5+C7H10_R5_4=C2H6+C7H9r_Olef_5	2.85E12	0.000	21462.2
C2H5+C7H10_R5_4=C2H6+C7H9r_Olef_6	2.85E12	0.000	21462.2
C2H5+C7H10_R5_4=C2H6+C7H9r_R5_9	1.25E12	0.000	15128.7
C2H5+C7H10_R5_5=C2H6+C7H9r_R5_10	9.30E11	0.000	15535.0

C2H5+C7H10_R5_5=C2H6+C7H9r_R5_9	4.65E11	0.000	15535.0
C2H5+C7H10_R5_6=C2H6+CC*cy(CCJCC*C)	2.85E12	0.000	21462.2
C2H5+C7H10_R5_6=C2H6+CC*cy(CCJC*CC)	2.85E12	0.000	21462.2
C2H5+C7H10_R5_6=C2H6+C7H9r_R5_5	1.25E12	0.000	15128.7
C2H5+C7H10_R5_9=C2H6+C7H9r_R5_1	2.85E12	0.000	21462.2
C2H5+C7H10_R5_9=C2H6+C7H9r_R5_16	4.97E12	0.000	18976.6
C2H5+C7H10_R5_9=C2H6+C7H9r_R5_15	1.42E12	0.000	21462.2
C2H5+C*CCCC*CC=C2H6+C*CCC*CCJC	2.69E12	0.000	13455.7
C2H5+C*CCCC*CC=C2H6+C*CCCCJC*C	1.25E12	0.000	15128.7
C2H5+C*CCCC*CC=C2H6+C*CCJCC*CC	2.69E12	0.000	13455.7
C2H5+C*CC(C)CC*C=C2H6+C7H11r_Olef	8.92E11	0.000	11997.8
C2H5+C*CC(C)CC*C=C2H6+C7H11r_Olef_23	4.97E12	0.000	18976.6
C2H5+C*CC(C)CC*C=C2H6+C7H11r_Olef_2	2.69E12	0.000	13455.7
C3H5-A+C*Ccy(CCC*CC)=C3H6+C7H9r_R5_17	1.89E13	0.000	32432.3
C3H5-A+C*Ccy(CCC*CC)=C3H6+C7H9r_R5_18	7.58E13	0.000	32432.3
C3H5-A+Ccy(C*CC*C(C)C)=C3H6+C7H9r_Olef_4	3.79E13	0.000	32432.3
C3H5-A+Ccy(C*CC*C(C)C)=C3H6+C7H9r_R5_22	3.32E13	0.000	26098.8
C3H5-A+Ccy(C*CCC*C(C))=C3H6+C7H9r_Olef_12	3.79E13	0.000	32432.3
C3H5-A+Ccy(C*CCC*C(C))=C3H6+C7H9r_R5_8	3.32E13	0.000	26098.8
C3H5-A+Ccy(CC(C)*CC*C)=C3H6+C7H9r_Olef_12	1.89E13	0.000	32432.3
C3H5-A+Ccy(CC(C)*CC*C)=C3H6+C7H9r_Olef_16	5.53E13	0.000	29946.7
C3H5-A+Ccy(CC(C)*CC*C)=C3H6+C7H9r_R5_1	1.66E13	0.000	26098.8
C3H5-A+CCcyCC*CC*C=C3H6+CJcCcyCC*CC*C	4.20E13	0.000	29516.5
C3H5-A+CCcyCC*CC*C=C3H6+CCJcyCC*CC*C	4.17E13	0.000	27652.3
!C3H5-A+CCcyCC*CC*C=C3H6+CCcyCJC*CC*C	1.44E13	0.000	32002.1
C3H5-A+Ccy(C*CC(C)*CC)=C3H6+C7H9r_Olef_4	3.79E13	0.000	32432.3
C3H5-A+Ccy(C*CC(C)*CC)=C3H6+C7H9r_Olef_5	1.66E13	0.000	26098.8
C3H5-A+Ccy(C*CC(C)*CC)=C3H6+C7H9r_Olef_6	1.66E13	0.000	26098.8
C3H5-A+Ccy(CC*C(C)C*C)=C3H6+C7H9r_Olef_2	1.66E13	0.000	26098.8
C3H5-A+Ccy(CC*C(C)C*C)=C3H6+C7H9r_Olef_3	5.53E13	0.000	29946.7
C3H5-A+Ccy(CC*C(C)C*C)=C3H6+C7H9r_Olef_4	1.89E13	0.000	32432.3
C3H5-A+CCcyC*CC*CC=C3H6+CJcCcyC*CC*CC	5.53E13	0.000	29946.7
!C3H5-A+CCcyC*CC*CC=C3H6+CCcyCJC*CC*C	3.79E13	0.000	32432.3
C3H5-A+CCcyC*CC*CC=C3H6+CC*cy(CCJC*CC)	3.58E13	0.000	24425.8
C3H5-A+CCcyC*CCC*C=C3H6+CJcCcyC*CCC*C	5.53E13	0.000	29946.7
C3H5-A+CCcyC*CCC*C=C3H6+CC*cy(CCJCC*C)	3.58E13	0.000	24425.8
!C3H5-A+CCcyC*CCC*C=C3H6+CCcyCJC*CC*C	3.79E13	0.000	32432.3
C3H5-A+Ccy(C*C(C)C*CC)=C3H6+C7H9r_Olef_12	3.79E13	0.000	32432.3
C3H5-A+Ccy(C*C(C)C*CC)=C3H6+C7H9r_R5_15	1.66E13	0.000	26098.8
C3H5-A+Ccy(C*C(C)C*CC)=C3H6+C7H9r_R5_2	1.66E13	0.000	26098.8
C3H5-A+Ccy(CC*CC*CC)=C3H6+CJcy(CC*CC*CC)	5.52E13	0.000	29946.7
C3H5-A+C7H10_R5_10=C3H6+CC*cy(CCJC*CC)	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_10=C3H6+C7H9r_R5_17	1.66E13	0.000	26098.8
C3H5-A+C7H10_R5_11=C3H6+C7H9r_R5_18	2.89E13	0.000	32002.1
C3H5-A+C7H10_R5_11=C3H6+C7H9r_R5_21	3.30E13	0.000	32432.3
C3H5-A+C7H10_R5_11=C3H6+C7H9r_R5_5	1.44E13	0.000	32002.1
C3H5-A+C7H10_R5_13=C3H6+C7H9r_Olef_6	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_13=C3H6+C7H9r_R5_10	1.66E13	0.000	26098.8
C3H5-A+C7H10_R5_13=C3H6+C7H9r_R5_22	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_15=C3H6+C7H9r_Olef_2	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_15=C3H6+C7H9r_R5_22	1.89E13	0.000	32432.3
C3H5-A+C7H10_R5_15=C3H6+C7H9r_R5_25	5.52E13	0.000	29946.7
C3H5-A+C7H10_R5_1=C3H6+C7H9r_R5_3	5.40E12	0.000	26505.1
C3H5-A+C7H10_R5_1=C3H6+C7H9r_R5_4	9.43E12	0.000	26074.9
C3H5-A+C7H10_R5_2=C3H6+C7H9r_R5_5	2.89E13	0.000	32002.1
C3H5-A+C7H10_R5_2=C3H6+C*Ccy(C*CCCJC)	3.30E13	0.000	32432.3
C3H5-A+C7H10_R5_2=C3H6+C7H9r_R5_7	2.89E13	0.000	32002.1
C3H5-A+C7H10_R5_3=C3H6+C7H9r_R5_2	3.79E13	0.000	32432.3

C3H5-A+C7H10_R5_3=C3H6+C7H9r_R5_4	1.66E13	0.000	26098.8
C3H5-A+C7H10_R5_3=C3H6+C7H9r_R5_8	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_4=C3H6+C7H9r_Olef_5	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_4=C3H6+C7H9r_Olef_6	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_4=C3H6+C7H9r_R5_9	1.66E13	0.000	26098.8
C3H5-A+C7H10_R5_5=C3H6+C7H9r_R5_10	1.24E13	0.000	26505.1
C3H5-A+C7H10_R5_5=C3H6+C7H9r_R5_9	6.19E12	0.000	26505.1
C3H5-A+C7H10_R5_6=C3H6+CC*cy(CCJCC*C)	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_6=C3H6+CC*cy(CCJC*CC)	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_6=C3H6+C7H9r_R5_5	1.66E13	0.000	26098.8
C3H5-A+C7H10_R5_9=C3H6+C7H9r_R5_1	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_9=C3H6+C7H9r_R5_16	5.52E13	0.000	29946.7
C3H5-A+C7H10_R5_9=C3H6+C7H9r_R5_15	1.89E13	0.000	32432.3
C3H5-A+C7H10_R5_8=C3H6+C7H9r_R5_12	5.53E13	0.000	29946.7
C3H5-A+C7H10_R5_8=C3H6+C7H9r_R5_1	3.79E13	0.000	32432.3
C3H5-A+C7H10_R5_8=C3H6+C7H9r_R5_2	1.89E13	0.000	32432.3
CH3+C*Ccy(CCC*CC)=CH4+C7H9r_R5_17	8.78E12	0.000	20171.6
CH3+C*Ccy(CCC*CC)=CH4+C7H9r_R5_18	3.51E13	0.000	20171.6
CH3+Ccy(CC*CC*CC)=CH4+CJcy(CC*CC*CC)	3.10E13	0.000	17686.0
CH3+Ccy(CC*C(C)C*C)=CH4+C7H9r_Olef_3	3.10E13	0.000	17686.0
CH3+Ccy(CC*C(C)C*C)=CH4+C7H9r_Olef_4	8.78E12	0.000	20171.6
CH3+Ccy(CC*C(C)C*C)=CH4+C7H9r_Olef_2	7.68E12	0.000	13838.1
CH3+Ccy(C*CC*C(C)C)=CH4+C7H9r_Olef_4	1.76E13	0.000	20171.6
CH3+Ccy(C*CC*C(C)C)=CH4+C7H9r_R5_22	1.54E13	0.000	13838.1
CH3+Ccy(C*CCC*C(C))=CH4+C7H9r_Olef_12	1.76E13	0.000	20171.6
CH3+Ccy(C*CCC*C(C))=CH4+C7H9r_R5_8	1.54E13	0.000	13838.1
CH3+CCcyCC*CC*C=CH4+CJcyCC*CC*C	2.36E13	0.000	17255.8
CH3+CCcyCC*CC*C=CH4+CCJcyCC*CC*C	2.22E13	0.000	15391.6
!CH3+CCcyCC*CC*C=CH4+CCcyCJC*CC*C	6.69E12	0.000	19741.4
CH3+Ccy(C*CC(C)*CC)=CH4+C7H9r_Olef_4	1.76E13	0.000	20171.6
CH3+Ccy(C*CC(C)*CC)=CH4+C7H9r_Olef_5	7.68E12	0.000	13838.1
CH3+Ccy(C*CC(C)*CC)=CH4+C7H9r_Olef_6	7.68E12	0.000	13838.1
CH3+CCcyC*CC*CC=CH4+CJcyC*CC*CC	3.10E13	0.000	17686.0
!CH3+CCcyC*CC*CC=CH4+CCcyCJC*CC*C	1.76E13	0.000	20171.6
CH3+CCcyC*CC*CC=CH4+CC*cy(CCJC*CC)	1.66E13	0.000	12165.1
CH3+CCcyC*CCC*C=CH4+CJcyC*CCC*C	3.10E13	0.000	17686.0
CH3+CCcyC*CCC*C=CH4+CC*cy(CCJCC*C)	1.66E13	0.000	12165.1
!CH3+CCcyC*CCC*C=CH4+CCcyCJC*CC*C	1.76E13	0.000	20171.6
CH3+Ccy(C*C(C)C*CC)=CH4+C7H9r_Olef_12	1.76E13	0.000	20171.6
CH3+Ccy(C*C(C)C*CC)=CH4+C7H9r_R5_15	7.68E12	0.000	13838.1
CH3+Ccy(C*C(C)C*CC)=CH4+C7H9r_R5_2	7.68E12	0.000	13838.1
CH3+Ccy(CC(C)*CC*C)=CH4+C7H9r_Olef_16	3.10E13	0.000	17686.0
CH3+Ccy(CC(C)*CC*C)=CH4+C7H9r_Olef_12	8.78E12	0.000	20171.6
CH3+Ccy(CC(C)*CC*C)=CH4+C7H9r_R5_1	7.68E12	0.000	13838.1
CH3+C7H10_R5_8=CH4+C7H9r_R5_12	3.10E13	0.000	17686.0
CH3+C7H10_R5_8=CH4+C7H9r_R5_1	1.76E13	0.000	20171.6
CH3+C7H10_R5_8=CH4+C7H9r_R5_2	8.78E12	0.000	20171.6
CH3+C7H10_R5_10=CH4+CC*cy(CCJC*CC)	1.76E13	0.000	20171.6
CH3+C7H10_R5_10=CH4+C7H9r_R5_17	7.68E12	0.000	13838.1
CH3+C7H10_R5_11=CH4+C7H9r_R5_18	1.34E13	0.000	19741.4
CH3+C7H10_R5_11=CH4+C7H9r_R5_21	1.76E13	0.000	20171.6
CH3+C7H10_R5_11=CH4+C7H9r_R5_5	6.69E12	0.000	19741.4
CH3+C7H10_R5_13=CH4+C7H9r_Olef_6	1.76E13	0.000	20171.6
CH3+C7H10_R5_13=CH4+C7H9r_R5_10	7.68E12	0.000	13838.1
CH3+C7H10_R5_13=CH4+C7H9r_R5_22	1.76E13	0.000	20171.6
CH3+C7H10_R5_15=CH4+C7H9r_Olef_2	1.76E13	0.000	20171.6
CH3+C7H10_R5_15=CH4+C7H9r_R5_22	8.78E12	0.000	20171.6
CH3+C7H10_R5_15=CH4+C7H9r_R5_25	3.10E13	0.000	17686.0

CH3+C7H10_R5_1=CH4+C7H9r_R5_3	2.87E12	0.000	14244.4
CH3+C7H10_R5_1=CH4+C7H9r_R5_4	4.37E12	0.000	13814.2
CH3+C7H10_R5_2=CH4+C7H9r_R5_5	1.34E13	0.000	19741.4
CH3+C7H10_R5_2=CH4+C*Ccy(C*CCCJC)	1.76E13	0.000	20171.6
CH3+C7H10_R5_2=CH4+C7H9r_R5_7	1.34E13	0.000	19741.4
CH3+C7H10_R5_3=CH4+C7H9r_R5_2	1.76E13	0.000	20171.6
CH3+C7H10_R5_3=CH4+C7H9r_R5_4	7.68E12	0.000	13838.1
CH3+C7H10_R5_3=CH4+C7H9r_R5_8	1.76E13	0.000	20171.6
CH3+C7H10_R5_4=CH4+C7H9r_Olef_5	1.76E13	0.000	20171.6
CH3+C7H10_R5_4=CH4+C7H9r_Olef_6	1.76E13	0.000	20171.6
CH3+C7H10_R5_4=CH4+C7H9r_R5_9	7.68E12	0.000	13838.1
CH3+C7H10_R5_5=CH4+C7H9r_R5_10	5.73E12	0.000	14244.4
CH3+C7H10_R5_5=CH4+C7H9r_R5_9	2.87E12	0.000	14244.4
CH3+C7H10_R5_6=CH4+CC*cy(CCJCC*C)	1.76E13	0.000	20171.6
CH3+C7H10_R5_6=CH4+CC*cy(CCJC*CC)	1.76E13	0.000	20171.6
CH3+C7H10_R5_6=CH4+C7H9r_R5_5	7.68E12	0.000	13838.1
CH3+C7H10_R5_9=CH4+C7H9r_R5_1	1.76E13	0.000	20171.6
CH3+C7H10_R5_9=CH4+C7H9r_R5_16	3.10E13	0.000	17686.0
CH3+C7H10_R5_9=CH4+C7H9r_R5_15	8.78E12	0.000	20171.6
H+C*Ccy(CCC*CC)=H2+C7H9r_R5_17	4.72E13	0.000	5903.3
H+C*Ccy(CCC*CC)=H2+C7H9r_R5_18	3.05E14	0.000	7170.0
H+C*cy(CCC*CCC)=H2+CJcy(C*CC*CCC)	2.01E14	0.000	6190.1
H+C*cy(CCC*CCC)=H2+C*cy(CCC*CCJC)	1.30E14	0.000	7074.4
H+C*cy(CCC*CCC)=H2+CJcy(C*CCC*CC)	1.30E14	0.000	7074.4
H+Ccy(CC*CCC*C)=H2+C7H9r_Olef_1	3.36E14	0.000	12595.3
H+Ccy(C*CC*(C)C)=H2+C7H9r_Olef_4	2.01E14	0.000	6190.1
H+Ccy(C*CC*(C)C)=H2+C7H9r_R5_22	1.46E14	0.000	9177.6
H+Ccy(C*CCC*(C)C)=H2+C7H9r_Olef_12	2.01E14	0.000	6190.1
H+Ccy(C*CCC*(C)C)=H2+C7H9r_R5_8	1.46E14	0.000	9177.6
H+CCcyCC*CC*C=H2+CJcyCC*CC*C	2.87E14	0.000	12499.7
H+CCcyCC*CC*C=H2+CCJcyCC*CC*C	2.33E14	0.000	9942.4
!H+CCcyCC*CC*C=H2+CCcyCJC*CC*C	4.39E13	0.000	5114.6
H+Ccy(C*CCCC*C)=H2+C7H9r_Olef	7.28E13	0.000	9177.6
H+Ccy(C*CC(C)*CC)=H2+C7H9r_Olef_4	2.01E14	0.000	6190.1
H+Ccy(C*CC(C)*CC)=H2+C7H9r_Olef_5	7.28E13	0.000	9177.6
H+Ccy(C*CC(C)*CC)=H2+C7H9r_Olef_6	7.28E13	0.000	9177.6
H+Ccy(CC*(C)C*(C))=H2+C7H9r_Olef_2	7.28E13	0.000	9177.6
H+Ccy(CC*(C)C*(C))=H2+C7H9r_Olef_3	3.36E14	0.000	12595.3
H+Ccy(CC*(C)C*(C))=H2+C7H9r_Olef_4	5.38E13	0.000	5401.4
H+CCcyC*CC*CC=H2+CJcyC*CC*CC	2.87E14	0.000	12499.7
!H+CCcyC*CC*CC=H2+CCcyCJC*CC*C	2.01E14	0.000	6190.1
H+CCcyC*CC*CC=H2+CC*cy(CCJC*CC)	1.59E14	0.000	7361.2
H+CCcyC*CCC*C=H2+CJcyC*CCC*C	2.87E14	0.000	12499.7
H+CCcyC*CCC*C=H2+CC*cy(CCJCC*C)	1.59E14	0.000	7361.2
!H+CCcyC*CCC*C=H2+CCcyCJC*CC*C	2.01E14	0.000	6190.1
H+Ccy(C*CC*CCC)=H2+CJcy(C*CC*CCC)	7.28E13	0.000	9177.6
H+Ccy(C*(C)C*(C))=H2+C7H9r_Olef_12	2.01E14	0.000	6190.1
H+Ccy(C*(C)C*(C))=H2+C7H9r_R5_15	7.28E13	0.000	9177.6
H+Ccy(C*(C)C*(C))=H2+C7H9r_R5_2	7.28E13	0.000	9177.6
H+Ccy(CC(C)*CC*(C))=H2+C7H9r_Olef_16	3.36E14	0.000	12595.3
H+Ccy(CC(C)*CC*(C))=H2+C7H9r_Olef_12	5.38E13	0.000	5401.4
H+Ccy(CC(C)*CC*(C))=H2+C7H9r_R5_1	7.28E13	0.000	9177.6
H+Ccy(CC*CC*CC)=H2+CJcy(CC*CC*CC)	3.36E14	0.000	12595.3
H+C7H10_R5_10=H2+CC*cy(CCJC*CC)	2.01E14	0.000	6190.1
H+C7H10_R5_10=H2+C7H9r_R5_177.28E13	0.000	9177.6	
H+C7H10_R5_11=H2+C7H9r_R5_181.30E14	0.000	7074.4	
H+C7H10_R5_11=H2+C7H9r_R5_212.33E14	0.000	9942.4	
H+C7H10_R5_11=H2+C7H9r_R5_5 4.39E13	0.000	5114.6	

H+C7H10_R5_13=H2+C7H9r_Olef_6	2.01E14	0.000	6190.1
H+C7H10_R5_13=H2+C7H9r_R5_107.28E13		0.000	9177.6
H+C7H10_R5_13=H2+C7H9r_R5_222.01E14		0.000	6190.1
H+C7H10_R5_15=H2+C7H9r_R5_224.72E13		0.000	5903.3
H+C7H10_R5_15=H2+C7H9r_R5_253.36E14		0.000	12595.3
H+C7H10_R5_15=H2+C7H9r_Olef_2	1.52E14	0.000	7170.0
H+C7H10_R5_1=H2+C7H9r_R5_3	1.99E14	0.000	9846.8
H+C7H10_R5_1=H2+C7H9r_R5_4	2.60E14	0.000	7074.4
H+C7H10_R5_2=H2+C7H9r_R5_5	1.30E14	0.000	7074.4
H+C7H10_R5_2=H2+C*ccy(C*CCCJC)	1.99E14	0.000	9846.8
H+C7H10_R5_2=H2+C7H9r_R5_7	1.30E14	0.000	7074.4
H+C7H10_R5_3=H2+C7H9r_R5_2	1.30E14	0.000	7074.4
H+C7H10_R5_3=H2+C7H9r_R5_4	7.28E13	0.000	9177.6
H+C7H10_R5_3=H2+C7H9r_R5_8	1.30E14	0.000	7074.4
H+C7H10_R5_4=H2+C7H9r_Olef_51.30E14		0.000	7074.4
H+C7H10_R5_4=H2+C7H9r_Olef_61.30E14		0.000	7074.4
H+C7H10_R5_4=H2+C7H9r_R5_9	7.28E13	0.000	9177.6
H+C7H10_R5_5=H2+C7H9r_R5_10	2.60E14	0.000	7074.4
H+C7H10_R5_5=H2+C7H9r_R5_9	2.01E14	0.000	6190.1
H+C7H10_R5_6=H2+CC*cy(CCJCC*C)	1.30E14	0.000	7074.4
H+C7H10_R5_6=H2+CC*cy(CCJC*CC)	1.30E14	0.000	7074.4
H+C7H10_R5_6=H2+C7H9r_R5_5	7.28E13	0.000	9177.6
H+C7H10_R5_8=H2+C7H9r_R5_12	3.36E14	0.000	12595.3
H+C7H10_R5_8=H2+C7H9r_R5_1	2.01E14	0.000	6190.1
H+C7H10_R5_8=H2+C7H9r_R5_2	5.38E13	0.000	5401.4
H+C7H10_R5_9=H2+C7H9r_R5_1	1.52E14	0.000	7170.0
H+C7H10_R5_9=H2+C7H9r_R5_15	4.72E13	0.000	5903.3
H+C7H10_R5_9=H2+C7H9r_R5_16	3.36E14	0.000	12595.3
H+C7H10_R6=H2+C7H9r_Olef	1.30E14	0.000	7074.4
H+C7H10_R6=H2+CJcy(C*CC*CCC)	1.30E14	0.000	7074.4
H+C7H10_R6=H2+C*cy(CC*CCCJC)	1.99E14	0.000	9846.8
H+Ccy(C*CCC*CC)=H2+CJcy(C*CCC*CC)	7.28E13	0.000	9177.6
OH+C*ccy(CCC*CC)=H2O+C7H9r_R5_17	2.60E5	2.300	-1362.3
OH+C*ccy(CCC*CC)=H2O+C7H9r_R5_18	1.04E6	2.300	-1362.3
OH+C*cy(CCC*CCC)=H2O+CJcy(C*CC*CCC)	5.20E5	2.300	-1362.3
OH+C*cy(CCC*CCC)=H2O+C*cy(CCC*CCJC)	5.20E5	2.300	-1362.3
OH+C*cy(CCC*CCC)=H2O+CJcy(C*CCC*CC)	5.20E5	2.300	-1362.3
OH+Ccy(CC*CCC*C)=H2O+Ccy(C*CCJCC*C)	2.60E5	2.300	-1362.3
OH+Ccy(CC*CCC*C)=H2O+Ccy(CCJC*CC*C)	5.20E5	2.300	-1362.3
OH+Ccy(CC*CC*CC)=H2O+Ccy(CCJC*CC*C)	5.20E5	2.300	-1362.3
OH+Ccy(CC*CC*CC)=H2O+Ccy(CJCC*CC*C)	2.60E5	2.300	-1362.3
OH+Ccy(C*CC*C(C)C)=H2O+C7H9r_Olef_4	5.20E5	2.300	-1362.3
OH+Ccy(C*CC*C(C)C)=H2O+C7H9r_R5_22	1.56E6	2.300	-1362.3
OH+Ccy(C*CCC*C(C))=H2O+C7H9r_Olef_12	5.20E5	2.300	-1362.3
OH+Ccy(C*CCC*C(C))=H2O+C7H9r_R5_8	1.56E6	2.300	-1362.3
OH+Ccy(CC(C)*CC*C)=H2O+C7H9r_Olef_12	2.60E5	2.300	-1362.3
OH+Ccy(CC(C)*CC*C)=H2O+C7H9r_R5_1	7.80E5	2.300	-1362.3
OH+CCcyCC*CC*C=H2O+CCcyCJC*CC*C	2.60E5	2.300	-1362.3
OH+Ccy(C*CCCC*C)=H2O+C7H9r_Olef	7.80E5	2.300	-1362.3
OH+Ccy(C*CCCC*C)=H2O+Ccy(C*CCCJC*C)	5.20E5	2.300	-1362.3
OH+Ccy(C*CCCC*C)=H2O+Ccy(C*CCJCC*C)	5.20E5	2.300	-1362.3
OH+Ccy(C*CC(C)*CC)=H2O+C7H9r_Olef_4	5.20E5	2.300	-1362.3
OH+Ccy(C*CC(C)*CC)=H2O+C7H9r_Olef_5	7.80E5	2.300	-1362.3
OH+Ccy(C*CC(C)*CC)=H2O+C7H9r_Olef_6	7.80E5	2.300	-1362.3
OH+Ccy(CC*C(C)C*C)=H2O+C7H9r_Olef_2	7.80E5	2.300	-1362.3
OH+Ccy(CC*C(C)C*C)=H2O+C7H9r_Olef_4	2.60E5	2.300	-1362.3
OH+CCcyC*CC*CC=H2O+CCcyCJC*CC*C	5.20E5	2.300	-1362.3
OH+CCcyC*CC*CC=H2O+CC*cy(CCJC*CC)	5.20E5	2.300	-1362.3

OH+CCcyC*CCC*C=H2O+CC*cy(CCJCC*C)	5.20E5	2.300	-1362.3
OH+CCcyC*CCC*C=H2O+CCcyCJC*CC*C	5.20E5	2.300	-1362.3
OH+Ccy(C*CC*CCC)=H2O+CJcy(C*CC*CCC)	7.80E5	2.300	-1362.3
OH+Ccy(C*CC*CCC)=H2O+Ccy(C*CCCJC*C)	5.20E5	2.300	-1362.3
OH+Ccy(C*CC*CCC)=H2O+Ccy(CJCC*CC*C)	5.20E5	2.300	-1362.3
OH+Ccy(C*(C)C*CC)=H2O+C7H9r_Olef_12	5.20E5	2.300	-1362.3
OH+Ccy(C*(C)C*CC)=H2O+C7H9r_R5_15	7.80E5	2.300	-1362.3
OH+Ccy(C*(C)C*CC)=H2O+C7H9r_R5_2	7.80E5	2.300	-1362.3
OH+C7H10_R5_10=H2O+CC*cy(CCJC*CC)	5.20E5	2.300	-1362.3
OH+C7H10_R5_10=H2O+C7H9r_R5_17	7.80E5	2.300	-1362.3
OH+C7H10_R5_11=H2O+C7H9r_R5_18	5.20E5	2.300	-1362.3
OH+C7H10_R5_11=H2O+C7H9r_R5_5	2.60E5	2.300	-1362.3
OH+C7H10_R5_13=H2O+C7H9r_Olef_6	5.20E5	2.300	-1362.3
OH+C7H10_R5_13=H2O+C7H9r_R5_10	7.80E5	2.300	-1362.3
OH+C7H10_R5_13=H2O+C7H9r_R5_22	5.20E5	2.300	-1362.3
OH+C7H10_R5_15=H2O+C7H9r_R5_22	2.60E5	2.300	-1362.3
OH+C7H10_R5_15=H2O+C7H9r_Olef_2	5.20E5	2.300	-1362.3
OH+C7H10_R5_1=H2O+C7H9r_R5_41.04E6	2.300	-1362.3	
OH+C7H10_R5_2=H2O+C7H9r_R5_55.20E5	2.300	-1362.3	
OH+C7H10_R5_2=H2O+C7H9r_R5_75.20E5	2.300	-1362.3	
OH+C7H10_R5_3=H2O+C7H9r_R5_25.20E5	2.300	-1362.3	
OH+C7H10_R5_3=H2O+C7H9r_R5_47.80E5	2.300	-1362.3	
OH+C7H10_R5_3=H2O+C7H9r_R5_85.20E5	2.300	-1362.3	
OH+C7H10_R5_4=H2O+C7H9r_Olef_5	5.20E5	2.300	-1362.3
OH+C7H10_R5_4=H2O+C7H9r_Olef_6	5.20E5	2.300	-1362.3
OH+C7H10_R5_4=H2O+C7H9r_R5_97.80E5	2.300	-1362.3	
OH+C7H10_R5_5=H2O+C7H9r_R5_10	1.04E6	2.300	-1362.3
OH+C7H10_R5_5=H2O+C7H9r_R5_95.20E5	2.300	-1362.3	
OH+C7H10_R5_6=H2O+CC*cy(CCJCC*C)	5.20E5	2.300	-1362.3
OH+C7H10_R5_6=H2O+CC*cy(CCJC*CC)	5.20E5	2.300	-1362.3
OH+C7H10_R5_6=H2O+C7H9r_R5_57.80E5	2.300	-1362.3	
OH+C7H10_R5_9=H2O+C7H9r_R5_15.20E5	2.300	-1362.3	
OH+C7H10_R5_9=H2O+C7H9r_R5_15	2.60E5	2.300	-1362.3
OH+C7H10_R5_8=H2O+C7H9r_R5_15.20E5	2.300	-1362.3	
OH+C7H10_R5_8=H2O+C7H9r_R5_22.60E5	2.300	-1362.3	
OH+C7H10_R6=H2O+C7H9r_Olef	5.20E5	2.300	-1362.3
OH+C7H10_R6=H2O+CJcy(C*CC*CCC)	5.20E5	2.300	-1362.3
OH+C*CCCC*CC=H2O+C*CCC*CCJC	5.20E5	2.300	-1362.3
OH+C*CCCC*CC=H2O+C*CCCCJC*C	7.80E5	2.300	-1362.3
OH+C*CCCC*CC=H2O+C*CCJCC*CC	5.20E5	2.300	-1362.3
OH+C*CC(C)CC*C=H2O+C7H11r_Olef	2.60E5	2.300	-1362.3
OH+C*CC(C)CC*C=H2O+C7H11r_Olef_2	5.20E5	2.300	-1362.3
OH+Ccy(C*CCC*CC)=H2O+CJcy(C*CCC*CC)	7.80E5	2.300	-1362.3
OH+Ccy(C*CCC*CC)=H2O+Ccy(C*CCCJC*C)	5.20E5	2.300	-1362.3
OH+Ccy(C*CCC*CC)=H2O+Ccy(CJCC*CC*C)	5.20E5	2.300	-1362.3
H02+C*Ccy(CCC*CC)=H2O2+C7H9r_R5_17	2.56E-2	4.400	13546.5
H02+C*Ccy(CCC*CC)=H2O2+C7H9r_R5_18	1.02E-1	4.400	13546.5
H02+C*cy(CCC*CCC)=H2O2+CJcy(C*CC*CCC)	5.12E-2	4.400	13546.5
H02+C*cy(CCC*CCC)=H2O2+C*cy(CCC*CCJC)	5.12E-2	4.400	13546.5
H02+C*cy(CCC*CCC)=H2O2+CJcy(C*CCC*CC)	5.12E-2	4.400	13546.5
H02+Ccy(CC*CCC*C)=H2O2+Ccy(C*CCJCC*C)	2.56E-2	4.400	13546.5
H02+Ccy(CC*CCC*C)=H2O2+Ccy(CCJC*CC*C)	5.12E-2	4.400	13546.5
H02+Ccy(CC*CC*CC)=H2O2+Ccy(CCJC*CC*C)	5.12E-2	4.400	13546.5
H02+Ccy(CC*CC*CC)=H2O2+Ccy(CJCC*CC*C)	2.56E-2	4.400	13546.5
H02+Ccy(CC*(C)C*C)=H2O2+C7H9r_Olef_4	2.56E-2	4.400	13546.5
H02+Ccy(CC*(C)C*C)=H2O2+C7H9r_Olef_2	7.68E-2	4.400	13546.5
H02+Ccy(C*CC*(C)C)=H2O2+C7H9r_Olef_4	5.12E-2	4.400	13546.5
H02+Ccy(C*CC*(C)C)=H2O2+C7H9r_R5_22	1.54E-1	4.400	13546.5

HO2+Ccy(C*CCC*(C))=H2O2+C7H9r_Olef_12 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CCC*(C))=H2O2+C7H9r_R5_8 1.54E-1 4.400 13546.5
 HO2+CCcyCC*CC*C=H2O2+CCcyCJC*CC*C 2.56E-2 4.400 13546.5
 HO2+Ccy(C*CCCC*(C))=H2O2+C7H9r_Olef 7.68E-2 4.400 13546.5
 HO2+Ccy(C*CCCC*(C))=H2O2+Ccy(C*CCCCJC*(C)) 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CCCC*(C))=H2O2+Ccy(C*CCJCC*(C)) 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CC(C)*CC)=H2O2+C7H9r_Olef_4 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CC(C)*CC)=H2O2+C7H9r_Olef_5 7.68E-2 4.400 13546.5
 HO2+Ccy(C*CC(C)*CC)=H2O2+C7H9r_Olef_6 7.68E-2 4.400 13546.5
 HO2+CCcyC*CC*CC=H2O2+CCcyCJC*CC*C 5.12E-2 4.400 13546.5
 HO2+CCcyC*CC*CC=H2O2+CC*cy(CCJC*CC) 5.12E-2 4.400 13546.5
 HO2+CCcyC*CCC*C=H2O2+CC*cy(CCJCC*C) 5.12E-2 4.400 13546.5
 HO2+CCcyC*CCC*C=H2O2+CCcyCJC*CC*C 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CC*CCC)=H2O2+CJcy(C*CC*CCC) 7.68E-2 4.400 13546.5
 HO2+Ccy(C*CC*CCC)=H2O2+Ccy(C*CCCJC*(C)) 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CC*CCC)=H2O2+Ccy(CJCC*CC*(C)) 5.12E-2 4.400 13546.5
 HO2+Ccy(C*(C)C*CC)=H2O2+C7H9r_Olef_12 5.12E-2 4.400 13546.5
 HO2+Ccy(C*(C)C*CC)=H2O2+C7H9r_R5_15 7.68E-2 4.400 13546.5
 HO2+Ccy(C*(C)C*CC)=H2O2+C7H9r_R5_2 7.68E-2 4.400 13546.5
 HO2+Ccy(CC(C)*CC*(C))=H2O2+C7H9r_Olef_12 2.56E-2 4.400 13546.5
 HO2+Ccy(CC(C)*CC*(C))=H2O2+C7H9r_R5_1 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_8=H2O2+C7H9r_R5_1 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_8=H2O2+C7H9r_R5_2 2.56E-2 4.400 13546.5
 HO2+C7H10_R5_10=H2O2+CC*cy(CCJC*CC) 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_10=H2O2+C7H9r_R5_17 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_11=H2O2+C7H9r_R5_18 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_11=H2O2+C7H9r_R5_5 2.56E-2 4.400 13546.5
 HO2+C7H10_R5_13=H2O2+C7H9r_Olef_6 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_13=H2O2+C7H9r_R5_10 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_13=H2O2+C7H9r_R5_22 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_15=H2O2+C7H9r_R5_22 2.56E-2 4.400 13546.5
 HO2+C7H10_R5_15=H2O2+C7H9r_Olef_2 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_1=H2O2+C7H9r_R5_4 1.02E-1 4.400 13546.5
 HO2+C7H10_R5_2=H2O2+C7H9r_R5_5 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_2=H2O2+C7H9r_R5_7 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_3=H2O2+C7H9r_R5_2 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_3=H2O2+C7H9r_R5_4 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_3=H2O2+C7H9r_R5_8 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_4=H2O2+C7H9r_Olef_5 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_4=H2O2+C7H9r_Olef_6 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_4=H2O2+C7H9r_R5_9 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_5=H2O2+C7H9r_R5_10 1.02E-1 4.400 13546.5
 HO2+C7H10_R5_5=H2O2+C7H9r_R5_9 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_6=H2O2+CC*cy(CCJCC*(C)) 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_6=H2O2+CC*cy(CCJC*CC) 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_6=H2O2+C7H9r_R5_5 7.68E-2 4.400 13546.5
 HO2+C7H10_R5_9=H2O2+C7H9r_R5_1 5.12E-2 4.400 13546.5
 HO2+C7H10_R5_9=H2O2+C7H9r_R5_15 2.56E-2 4.400 13546.5
 HO2+C7H10_R6=H2O2+C7H9r_Olef 5.12E-2 4.400 13546.5
 HO2+C7H10_R6=H2O2+CJcy(C*CC*CCC) 5.12E-2 4.400 13546.5
 HO2+C*CCCC*CC=H2O2+C*CCC*CCJC 5.12E-2 4.400 13546.5
 HO2+C*CCCC*CC=H2O2+C*CCCCJC*(C) 7.68E-2 4.400 13546.5
 HO2+C*CCCC*CC=H2O2+C*CCJCC*CC 5.12E-2 4.400 13546.5
 HO2+C*CC(C)CC*(C)=H2O2+C7H11r_Olef 2.56E-2 4.400 13546.5
 HO2+C*CC(C)CC*(C)=H2O2+C7H11r_Olef_2 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CCC*CC)=H2O2+CJcy(C*CCC*CC) 7.68E-2 4.400 13546.5
 HO2+Ccy(C*CCC*CC)=H2O2+Ccy(C*CCCJC*(C)) 5.12E-2 4.400 13546.5
 HO2+Ccy(C*CCC*CC)=H2O2+Ccy(CJCC*CC*(C)) 5.12E-2 4.400 13546.5

C7H11r_Olef_10=C7H11r_Olef_13	7.20E12	0.000	54778.8
C7H11r_Olef_15=C7H11r_Olef_14	4.80E12	0.000	57646.8
C7H11r_Olef_2=C7H11r_Olef_237	2.0E12	0.000	55448.0
C7H11r_Olef_9=C7H11r_Olef_142	4.0E12	0.000	59319.8
C7H11r_Olef_9=C7H11r_Olef_152	4.0E12	0.000	51600.1
CCC*CC*CCJ=C7H11r_Olef_29	7.20E12	0.000	54778.8
C7H11r_Olef_14=C7H11r_Olef	4.50E11	0.000	33794.6
C7H11r_Olef_15=C7H11r_Olef_17	4.50E11	0.000	37642.5
C7H11r_Olef_15=C7H11r_Olef_18	9.00E11	0.000	46772.3
C7H11r_Olef_2=C7H11r_Olef_3	1.50E11	0.000	28608.3
C7H11r_Olef_3=C7H11r_Olef_103	0.00E11	0.000	35204.7
C7H11r_Olef_3=C7H11r_Olef_7	1.50E11	0.000	33794.6
C7H11r_Olef_9=C7H11r_Olef	3.00E11	0.000	42924.4
C7H11r_Olef_10=C7H11r_Olef_12	5.55E10	0.000	30639.8
C7H11r_Olef_15=C7H11r_Olef_73	7.0E10	0.000	25118.9
C7H11r_Olef_2=C7H11r_Olef_5	5.55E10	0.000	30639.8
C7H11r_Olef_9=C7H11r_Olef_7	1.85E10	0.000	26791.9
CCC*CC*CCJ=C7H11r_Olef_27	1.11E11	0.000	39769.6
C7H11r_Olef_15=C7H11r_Olef_20	6.87E9	0.000	29636.0
C7H11r_Olef_3=C7H11r_Olef_9	2.29E9	0.000	25788.1
CCC*CC*CCJ=CC*CC*CCJC	4.58E9	0.000	24115.1
C7H11r_Olef_13=C7H11r_R5_2	7.48E10	0.000	14483.4
C7H11r_Olef_14=C7H11r_R5_13	3.74E10	0.000	24712.6
C7H11r_Olef_14=C7H11r_R5_16	3.74E10	0.000	24617.0
C7H11r_Olef_15=C7H11r_R5_7	3.74E10	0.000	21533.9
C7H11r_Olef_20=C7H11r_R5_8	7.48E10	0.000	16443.2
C7H11r_Olef_23=C7H11r_R5_19	7.48E10	0.000	17662.1
C7H11r_Olef_29=C7H11r_R5_41	7.48E10	0.000	19143.9
C7H11r_Olef_3=C7H11r_R5_48	3.74E10	0.000	21892.4
C7H11r_Olef_9=C7H11r_R5_6	3.74E10	0.000	21892.4
C7H11r_Olef=Ccy(C*CCCCJC)	5.04E08	0.700	20246
C7H11r_Olef_12=Ccy(C*CCCCCJ)	1.04E10	0.000	7648.0
C7H11r_Olef_13=CJcy(C*CCCC)	1.04E10	0.000	7648.0
C7H11r_Olef_17=Ccy(CJC*CCCC)	1.04E10	0.000	7648.0
C7H11r_Olef_18=C*cy(CCCJCCC)	1.04E10	0.000	10372.6
C7H11r_Olef_2=Ccy(CC*CCCCJ)	5.04E08	0.700	20246
C*CCC*CCJC=C7H11r_R5_17	1.40E10	0.000	16759.6
C7H11r_Olef=C7H11r_R5_20	1.40E10	0.000	16855.2
C7H11r_Olef_12=C7H11r_R5_5	2.80E10	0.000	9780.8
C7H11r_Olef_13=C7H11r_R5_3	2.80E10	0.000	9780.8
C7H11r_Olef_17=C7H11r_R5_12	2.80E10	0.000	9780.8
C7H11r_Olef_18=C7H11r_R5_11	2.80E10	0.000	9804.7
C*CCJCC*CC=C7H11r_R5_35	2.80E10	0.000	16520.6
C7H11r_Olef_2=C7H11r_R5_17	1.40E10	0.000	16855.2
C7H11r_Olef_27=CJcy(CCC*CCC)	3.90E9	0.000	10109.7
C7H11r_Olef_29=CJcy(CC*CCCC)	3.90E9	0.000	10085.8
C4H6+C3H5-A=C7H11r_Olef_23	1.46E12	0.000	18331.3
DUP			
C4H6+C3H5-A=C7H11r_Olef_23	1.46E12	0.000	18331.3
DUP			
C*Ccy(CCC*CC)+H=C7H11r_R5_355	5.56E13	0.000	3847.9
C*Ccy(CCC*CC)+H=C7H11r_R5_366	4.46E13	0.000	5377.5
C*cy(CCC*CCC)+H=C*cy(CCCJCCC)	6.75E13	0.000	4803.9
C*cy(CCC*CCC)+H=Ccy(CJCC*CCC)	6.28E13	0.000	3250.4
C*cy(CCC*CCC)+H=C*cy(CCCCJCC)	6.75E13	0.000	4803.9
Ccy(CC*CCC*C)+H=Ccy(CC*CCCCJ)	1.35E14	0.000	4803.9
DUP			
Ccy(CC*CCC*C)+H=Ccy(CC*CCCCJ)	1.35E14	0.000	4803.9

DUP			
Ccy (CC*CCC*C) +H=Ccy (CC*CCCJC)	1.35E14	0.000	4803.9
DUP			
Ccy (CC*CCC*C) +H=Ccy (CC*CCCCJ)	1.35E14	0.000	4803.9
DUP			
Ccy (C*CCCC*C) +H=Ccy (CC*CCCCJ)	2.64E13	0.000	6166.2
Ccy (C*CCCC*C) +H=Ccy (C*CCCCCJ)	6.11E13	0.000	3704.5
Ccy (C*CCCC*C) +H=Ccy (CJC*CCCC)	6.81E13	0.000	3250.4
Ccy (C*CCCC*C) +H=Ccy (C*CCCCJC)	8.20E13	0.000	5377.5
Ccy (CC*CC*CC) +H=Ccy (CCJC*CCC)	6.11E13	0.000	3704.5
DUP			
Ccy (CC*CC*CC) +H=Ccy (CCJCC*CC)	8.20E13	0.000	5377.5
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_50	6.81E13	0.000	3250.4
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_48	6.11E13	0.000	3704.5
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_60	8.20E13	0.000	5377.5
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_51	2.64E13	0.000	6166.2
DUP			
Ccy (C*CC*C (C) C) +H=C7H11r_R5_57	1.85E14	0.000	4780.0
Ccy (C*CC*C (C) C) +H=C7H11r_R5_50	3.24E13	0.000	4517.1
Ccy (C*CCC*C (C)) +H=C7H11r_R5_23	1.36E14	0.000	3250.4
Ccy (C*CCC*C (C)) +H=C7H11r_R5_52	5.28E13	0.000	6166.2
Ccy (CC (C) *CC*C) +H=C7H11r_R5_25	9.27E13	0.000	4780.0
DUP			
Ccy (CC (C) *CC*C) +H=C7H11r_R5_6	6.11E13	0.000	3704.5
DUP			
Ccy (CC (C) *CC*C) +H=C7H11r_R5_52	8.20E13	0.000	5377.5
DUP			
Ccy (CC (C) *CC*C) +H=C7H11r_R5_73	1.62E13	0.000	4517.1
DUP			
CCcyCC*CC*C+H=C7H11r_R5_74	1.64E14	0.000	5377.5
DUP			
CCcyCC*CC*C+H=C7H11r_R5_75	1.22E14	0.000	3704.5
DUP			
CCcyCC*CC*C+H=C7H11r_R5_74	1.64E14	0.000	5377.5
DUP			
CCcyCC*CC*C+H=C7H11r_R5_75	1.22E14	0.000	3704.5
DUP			
Ccy (C*CC (C) *CC) +H=C7H11r_R5_48	1.62E13	0.000	4517.1
Ccy (C*CC (C) *CC) +H=C7H11r_R5_46	6.81E13	0.000	3250.4
Ccy (C*CC (C) *CC) +H=C7H11r_R5_57	9.27E13	0.000	4780.0
Ccy (C*CC (C) *CC) +H=C7H11r_R5_60	2.64E13	0.000	6166.2
Ccy (CC*C (C) C*C) +H=C7H11r_R5_48	6.11E13	0.000	3704.5
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_60	8.20E13	0.000	5377.5
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_50	6.81E13	0.000	3250.4
DUP			
Ccy (CC*C (C) C*C) +H=C7H11r_R5_51	2.64E13	0.000	6166.2
DUP			
CCcyC*CC*CC+H=C7H11r_R5_37	8.20E13	0.000	5377.5
CCcyC*CC*CC+H=C7H11r_R5_38	9.27E13	0.000	4780.0
CCcyC*CC*CC+H=C7H11r_R5_7	6.11E13	0.000	3704.5
CCcyC*CC*CC+H=C7H11r_R5_75	1.62E13	0.000	4517.1
CCcyC*CCC*C+H=C7H11r_R5_37	8.20E13	0.000	5377.5

CCcyC*CCC*C+H=C7H11r_R5_44	6.11E13	0.000	3704.5
CCcyC*CCC*C+H=C7H11r_R5_74	2.64E13	0.000	6166.2
CCcyC*CCC*C+H=C7H11r_R5_7	6.81E13	0.000	3250.4
Ccy(C*CC*CCC)+H=Ccy(CCJC*CCC)	1.62E13	0.000	4517.1
Ccy(C*CC*CCC)+H=Ccy(CJC*CCCC)	6.11E13	0.000	3704.5
Ccy(C*CC*CCC)+H=Ccy(CJCC*CCC)	9.27E13	0.000	4780.0
Ccy(C*CC*CCC)+H=Ccy(C*CCCJCC)	8.20E13	0.000	5377.5
Ccy(C*C(C)C*CC)+H=C7H11r_R5_23	6.11E13	0.000	3704.5
Ccy(C*C(C)C*CC)+H=C7H11r_R5_24	8.20E13	0.000	5377.5
Ccy(C*C(C)C*CC)+H=C7H11r_R5_25	2.99E13	0.000	5568.7
Ccy(C*C(C)C*CC)+H=C7H11r_R5_6	1.80E13	0.000	4063.0
Ccy(CC(C)*CC*C)+H=C7H11r_R5_6	6.11E13	0.000	3704.5
DUP			
Ccy(CC(C)*CC*C)+H=C7H11r_R5_25	9.27E13	0.000	4780.0
DUP			
Ccy(CC(C)*CC*C)+H=C7H11r_R5_52	8.20E13	0.000	5377.5
DUP			
Ccy(CC(C)*CC*C)+H=C7H11r_R5_73	1.62E13	0.000	4517.1
DUP			
Ccy(CC*CC*CC)+H=Ccy(CCJC*CCC)	6.11E13	0.000	3704.5
DUP			
Ccy(CC*CC*CC)+H=Ccy(CCJCC*CC)	8.20E13	0.000	5377.5
DUP			
Ccy(CC*CC*CC)+H=Ccy(CCC*CCJC)	6.11E13	0.000	3704.5
C7H10_R5_8+H=C7H11r_R5_17	1.71E13	0.000	6190.1
DUP			
C7H10_R5_8+H=C7H11r_R5_16	6.75E13	0.000	4803.9
DUP			
C7H10_R5_8+H=C7H11r_R5_25	6.28E13	0.000	3250.4
DUP			
C7H10_R5_8+H=C7H11r_R5_43	6.75E13	0.000	4803.9
DUP			
C7H10_R5_1+H=C7H11r_R5_3	5.06E13	0.000	6739.8
DUP			
C7H10_R5_1+H=C7H11r_R5_3	5.06E13	0.000	6739.8
DUP			
C7H10_R5_1+H=C7H11r_R5_54	1.12E14	0.000	2294.4
C7H10_R5_10+H=C7H11r_R5_13	6.75E13	0.000	4803.9
DUP			
C7H10_R5_10+H=C7H11r_R5_13	6.75E13	0.000	4803.9
DUP			
C7H10_R5_10+H=C7H11r_R5_35	1.79E13	0.000	5616.5
C7H10_R5_10+H=C7H11r_R5_38	7.62E13	0.000	4206.4
C7H10_R5_11+H=C7H11r_R5_32	5.56E13	0.000	3847.9
DUP			
C7H10_R5_11+H=C7H11r_R5_33	6.46E13	0.000	5377.5
DUP			
C7H10_R5_11+H=C7H11r_R5_41	6.75E13	0.000	4803.9
DUP			
C7H10_R5_11+H=C7H11r_R5_32	5.56E13	0.000	3847.9
DUP			
C7H10_R5_11+H=C7H11r_R5_33	6.46E13	0.000	5377.5
DUP			
C7H10_R5_11+H=C7H11r_R5_41	6.75E13	0.000	4803.9
DUP			
C7H10_R5_13+H=C7H11r_R5_20	1.71E13	0.000	6190.1
C7H10_R5_13+H=C7H11r_R5_47	7.62E13	0.000	4206.4
C7H10_R5_13+H=C7H11r_R5_57	6.28E13	0.000	3250.4

C7H10_R5_13+H=C7H11r_R5_59	1.79E13	0.000 5616.5
DUP		
C7H10_R5_13+H=C7H11r_R5_59	1.79E13	0.000 5616.5
DUP		
C7H10_R5_15+H=C7H11r_R5_59	8.20E13	0.000 5377.5
DUP		
C7H10_R5_15+H=C7H11r_R5_50	5.61E13	0.000 2294.4
DUP		
C7H10_R5_15+H=C7H11r_R5_63	2.53E13	0.000 6739.8
DUP		
C7H10_R5_15+H=C7H11r_R5_64	6.11E13	0.000 3704.5
DUP		
C7H10_R5_15+H=C7H11r_R5_50	5.61E13	0.000 2294.4
DUP		
C7H10_R5_15+H=C7H11r_R5_59	8.20E13	0.000 5377.5
DUP		
C7H10_R5_15+H=C7H11r_R5_63	2.53E13	0.000 6739.8
DUP		
C7H10_R5_15+H=C7H11r_R5_64	6.11E13	0.000 3704.5
DUP		
C7H10_R5_2+H=C7H11r_R5_2	6.81E13	0.000 3250.4
C7H10_R5_2+H=C7H11r_R5_41	2.64E13	0.000 6166.2
DUP		
C7H10_R5_2+H=C7H11r_R5_41	2.64E13	0.000 6166.2
DUP		
C7H10_R5_2+H=C7H11r_R5_55	5.03E13	0.000 2748.5
C7H10_R5_2+H=C7H11r_R5_56	7.85E13	0.000 5951.1
C7H10_R5_3+H=C7H11r_R5_43	2.64E13	0.000 6166.2
DUP		
C7H10_R5_3+H=C7H11r_R5_23	5.61E13	0.000 2294.4
C7H10_R5_3+H=C7H11r_R5_43	2.64E13	0.000 6166.2
DUP		
C7H10_R5_3+H=C7H11r_R5_5	2.53E13	0.000 6739.8
C7H10_R5_3+H=C7H11r_R5_54	6.81E13	0.000 3250.4
C7H10_R5_4+H=C7H11r_R5_12	2.53E13	0.000 6739.8
C7H10_R5_4+H=C7H11r_R5_46	5.61E13	0.000 2294.4
C7H10_R5_4+H=C7H11r_R5_47	9.27E13	0.000 4780.0
C7H10_R5_4+H=C7H11r_R5_8	1.62E13	0.000 4517.1
DUP		
C7H10_R5_4+H=C7H11r_R5_8	1.62E13	0.000 4517.1
DUP		
C7H10_R5_5+H=C7H11r_R5_11	3.42E13	0.000 6190.1
DUP		
C7H10_R5_5+H=C7H11r_R5_11	3.42E13	0.000 6190.1
DUP		
C7H10_R5_5+H=C7H11r_R5_47	1.26E14	0.000 3250.4
C7H10_R5_6+H=C7H11r_R5_13	8.20E13	0.000 5377.5
DUP		
C7H10_R5_6+H=C7H11r_R5_13	8.20E13	0.000 5377.5
DUP		
C7H10_R5_6+H=C7H11r_R5_55	6.11E13	0.000 3704.5
C7H10_R5_6+H=C7H11r_R5_32	2.64E13	0.000 6166.2
C7H10_R5_6+H=C7H11r_R5_7	6.81E13	0.000 3250.4
C7H10_R5_9+H=C7H11r_R5_16	8.20E13	0.000 5377.5
DUP		
C7H10_R5_9+H=C7H11r_R5_6	5.61E13	0.000 2294.4
DUP		
C7H10_R5_9+H=C7H11r_R5_27	2.53E13	0.000 6739.8

DUP
C7H10_R5_9+H=C7H11r_R5_28 6.11E13 0.000 3704.5
DUP
C7H10_R5_8+H=C7H11r_R5_16 6.75E13 0.000 4803.9
DUP
C7H10_R5_8+H=C7H11r_R5_17 1.71E13 0.000 6190.1
DUP
C7H10_R5_8+H=C7H11r_R5_25 6.28E13 0.000 3250.4
DUP
C7H10_R5_8+H=C7H11r_R5_43 6.75E13 0.000 4803.9
DUP
C7H10_R5_9+H=C7H11r_R5_16 8.20E13 0.000 5377.5
DUP
C7H10_R5_9+H=C7H11r_R5_6 5.61E13 0.000 2294.4
DUP
C7H10_R5_9+H=C7H11r_R5_27 2.53E13 0.000 6739.8
DUP
C7H10_R5_9+H=C7H11r_R5_28 6.11E13 0.000 3704.5
DUP
C7H10_R6+H=CJcy (C*CCCC) 6.11E13 0.000 3704.5
C7H10_R6+H=CJcy (CC*CCCC) 2.53E13 0.000 6739.8
C7H10_R6+H=C*cy (CCCJCCC) 8.20E13 0.000 5377.5
C7H10_R6+H=Ccy (CJC*CCCC) 5.61E13 0.000 2294.4
Ccy (C*CCC*CC) +H=Ccy (C*CCCCJC) 6.75E13 0.000 4803.9
Ccy (C*CCC*CC) +H=Ccy (CJCC*CCC) 7.62E13 0.000 4206.4
Ccy (C*CCC*CC) +H=Ccy (C*CCCJCC) 6.75E13 0.000 4803.9
Ccy (C*CCC*CC) +H=Ccy (CCJCC*CC) 1.79E13 0.000 5616.5
C7H11r_R5_48=Ccy (C*CCC*C) +CH3 2.61E14 0.000 39363.3
C7H11r_R5_25=CH3+Ccy (C*CC*CC) 1.40E13 0.000 26720.2
C7H11r_R5_43=C*cy (CC*CCC) +CH3 2.59E13 0.000 27126.5
C7H11r_R5_6=Ccy (C*CCC*C) +CH3 1.15E14 0.000 38837.5
C7H11r_R5_74=C2H5+C5H6 1.86E13 0.000 25047.2
C7H11r_R5_60=CH3+Ccy (C*CC*CC) 2.59E13 0.000 27126.5
C7H11r_R5_50=CH3+Ccy (C*CC*CC) 2.61E14 0.000 39363.3
C7H11r_R5_51=CH3+Ccy (CC*CC*C) 5.17E13 0.000 27126.5
C7H11r_R5_52=CH3+Ccy (C*CCC*C) 2.59E13 0.000 27126.5
C7H11r_R5_59=C*cy (CCC*CC) +CH3 4.66E13 0.000 30424.7
C7H11r_R5_8=C*cy (CC*CCC) +CH3 2.61E14 0.000 39363.3
Ccy (CC*CCCCJ) =CH3+cy (C*CC*CCC) 2.59E13 0.000 27126.5
Ccy (CCJC*CCC) =CH3+cy (C*CC*CCC) 2.61E14 0.000 39363.3
!Ccy (CCJCC*CC) =CH3+cy (C*CCC*CC) 4.66E13 0.000 30424.7
C7H9r_Olef_2=fulvene+CH3 1.45E14 0.000 36065.1
C7H9r_R5_1=>fulvene+CH3 1.45E14 0.000 36065.1
Ccy (CCJC*CC*C) =CH3+C6H6 2.89E14 0.000 36065.1
C*CCJCCC+HO2=C6H12O2_Olef_1 3.35E10 0.600 -2105.6
DUP
C*CCJCCC+HO2=C6H12O2_Olef_1 3.35E10 0.600 -2105.6
DUP
C*CCJCCC+HO2=C6H12O2_Olef_2 3.35E10 0.600 -2105.6
DUP
C*CCJCCC+HO2=C6H12O2_Olef_2 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+HO2=C6H12O3_Olef 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+HO2=C6H12O3_Olef 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+HO2=C6H12O3_Olef_2 3.35E10 0.600 -2105.6
DUP

C6H11Or_Olef_3+H2O=C6H12O3_Olef_2 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+H2O=C6H12O3_Olef 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+H2O=C6H12O3_Olef 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+H2O=C6H12O3_Olef_2 3.35E10 0.600 -2105.6
DUP
C6H11Or_Olef_3+H2O=C6H12O3_Olef_2 3.35E10 0.600 -2105.6
DUP
C5H6O2_Olef=>C5H5O+OH 1.59E20 -1.500 42857.5
C5H8O2_R5=>C5H7Or_R5+OH 1.59E20 -1.500 42857.5
C6H12O2_Olef_1=>CCCC*CCOJ+OH 1.59E20 -1.500 42857.5
C6H12O2_Olef_2=>C*CC(OJ)CCC+OH 1.59E20 -1.500 42857.5
C6H12O3_Olef=>C6H11O2r_4+OH 1.59E20 -1.500 42857.5
C6H12O3_Olef_2=>CC(OH)CC*CCOJ+OH 1.59E20 -1.500 42857.5
C5H7Or_R5=C*CCJCC*O 6.00E13 0.220 14098.6
C6H11O2r_4=C2H3CHO+C3H6OH2-19.00E13 0.220 14098.6
C*CC(OJ)CCC=NC3H7+C2H3CHO 9.00E13 0.220 14098.6
CC(OH)CC*CCOJ=CC(OH)CC*CC*O+H 3.52E10 1.000 18548.8
C6H11O2r_4=C6H10O2_Olef_3+H 1.76E10 1.000 18548.8
C*CC(OJ)CCC=C6H10O_Olef+H 1.76E10 1.000 18548.8
CCCC*CCOJ=C6H10O_Olef_11+H 3.52E10 1.000 18548.8
CC(OH)CC*CCOJ=C5H9Or_Olef+CH2O 8.10E14 0.000 23890.4
C6H11O2r_4=C2H3+C4H8O2 8.10E14 0.000 23890.4
C*CC(OJ)CCC=NC3H7CHO+C2H3 8.10E14 0.000 23890.4
CCCC*CCOJ=C5H9r_Olef_2+CH2O 8.10E14 0.000 23890.4
O2+CJcy(CC*CC*C)=C6H7O2r_Olef_3 5.20E11 0.230 -1579.8
O2+CJcy(CCC*CC)=COOJcy(CCC*CC) 5.20E11 0.230 -1579.8
O2+CJcy(CCCCC)=C(OOJ)cy(CCCCC) 5.20E11 0.230 -1579.8
O2+Ccy(CCCJCC)=C6H11O2r_R5_83.02E15 -0.920 -129.1
DUP
O2+Ccy(CCCJCC)=C6H11O2r_R5_83.02E15 -0.920 -129.1
DUP
O2+Ccy(CCCJCC)=C6H11O2r_R5_83.02E15 -0.920 -129.1
DUP
O2+Ccy(CCCJCC)=C6H11O2r_R5_83.02E15 -0.920 -129.1
DUP
O2+cy(C*CCCJCC)=JOOcy(CCC*CCC) 3.02E15 -0.920 -129.1
O2+C*cy(CCJC*CC)=C6H7O2r_Olef_7 2.90E7 1.590 1080.3
O2+C*cy(CCJC*CC)=C6H7O2r_R5_1 2.90E7 1.590 1080.3
O2+C*cy(CCJC*CC)=C6H7O2r_R5_2 2.90E7 1.590 1080.3
O2+C*cy(CCJCC*C)=C6H7O2r_Olef 2.90E7 1.590 1080.3
O2+C*cy(CCJCC*C)=C6H7O2r_R5 2.90E7 1.590 1080.3
O2+Ccy(CCJC*CC)=C6H9O2r_R5 2.90E7 1.590 1080.3
O2+Ccy(CCJC*CC)=C6H9O2r_R5_12.90E7 1.590 1080.3
O2+Ccy(CJC*CC*C)=C6H7O2r_Olef_4 2.90E7 1.590 1080.3
O2+Ccy(CJC*CC*C)=C6H7O2r_Olef_5 2.90E7 1.590 1080.3
O2+Ccy(CJC*CC*C)=C6H7O2r_Olef_6 2.90E7 1.590 1080.3
O2+cy(C*CC*CCJC)=C6H7O2r_Olef_1 5.80E7 1.590 1080.3
O2+cy(C*CC*CCJC)=C6H7O2r_Olef_2 5.80E7 1.590 1080.3
O2+cy(C*CCJCCC)=C6H9O2r_R6 5.80E7 1.590 1080.3
C6H9O2r_R5=C6H9O2r_R5_3 1.76E9 0.780 21849.4
C(OOJ)cy(CCCCC)=C6H11O2r_R5_11 1.64E11 0.130 19468.9
C6H11O2r_R5_8=C6H11O2r_R5_2 1.64E11 0.130 19468.9
C6H9O2r_R6=C6H9O2r_R6_1 1.64E11 0.130 19468.9
C6H11O2r_R5_8=C6H11O2r_R5_7 1.82E7 1.190 14999.6
C6H9O2r_R5=C6H9O2r_R5_4 1.12E5 2.010 12124.5

C6H9O2r_R5_1=C6H9O2r_R5_2 5.61E4 2.010 12124.5
 COOJcy(CCC*CC)=CPcy(CCJC*CC) 0.56E5 2.010 12124.5 ! RDB: /2 to
 match CPD profile
 C6H7O2r_Olef_6=fulvene+HO2 8.66E9 0.930 29799.3
 C6H11O2r_R5_8=C6H10_R5+HO2 5.77E9 0.930 29799.3
 C6H11O2r_R5_8=Ccy(CCC*CC)+HO2 5.77E9 0.930 29799.3
 C6H9O2r_R5_1=Ccy(CC*CC*C)+HO2 5.77E9 0.930 29799.3
 C6H9O2r_R6=cy(C*CC*CCC)+HO2 5.77E9 0.930 29799.3
 JOOcy(CCC*CCC)=cy(C*CCC*CC)+HO2 5.77E9 0.930 29799.3
 C(OOJ)cy(CCCCC)=C*cy(CCCCC) +HO2 2.88E9 0.930 29799.3
 C6H9O2r_R5=Ccy(C*CC*CC)+HO2 2.88E9 0.930 29799.3
 COOJcy(CCC*CC)=C*cy(CCC*CC)+HO2 2.88E9 0.930 29799.3
 C6H7O2r_Olef_2=C6H6+HO2 3.16E10 0.637 27578.2
 C6H7O2r_R5=fulvene+HO2 3.16E10 0.637 27578.2
 C6H7O2r_R5_2=fulvene+HO2 3.16E10 0.637 27578.2
 JOOcy(CCC*CCC)=cy(C*CC*CCC)+HO2 3.16E10 0.637 27578.2
 C6H11O2r_R5_11=cy(C*CCCC)+CH2O2H 14.50E13 0.000 26839.7 ! RDB x2
 to match cy(C*CCCC) profile
 C6H11O2r_R5_2=CH3+C5H8O2_R5 4.66E13 0.000 30424.7
 C6H9O2r_R5_4=CH3+C5H6O2_Olef 2.61E14 0.000 39363.3
 CPcy(CCJC*CC)=C5H6+CH2O2H 4.06E14 0.000 35778.3 ! Bugler values
 (5.82E+05 2.4 22790)do not take into account resonance stablization!
 CPC*CCJC*C=CPcy(CCJC*CC) 3.74E10 0.000 21964.1
 DUP
 CPC*CCJC*C=CPcy(CCJC*CC) 3.74E10 0.000 23493.7
 DUP
 C*CCJCCC+HO2=C6H12O2_Olef_2 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCC+HO2=C6H12O2_Olef_2 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCC+HO2=C6H12O2_Olef_1 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCC+HO2=C6H12O2_Olef_1 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCCP+HO2=C6H12O4_Olef_20 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCCP+HO2=C6H12O4_Olef_20 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCCP+HO2=C6H12O4_Olef_23 3.35E10 0.600 -2105.6
 DUP
 C*CCJCCCP+HO2=C6H12O4_Olef_23 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_15 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_15 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_12 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_12 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_12 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_12 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_15 3.35E10 0.600 -2105.6
 DUP
 C6H11O2r_14+HO2=C6H12O4_Olef_15 3.35E10 0.600 -2105.6
 DUP

C6H1102r_20+HO2=C6H12O4_Olef_15	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_15	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_15	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_15	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_18	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_18	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_18	3.35E10	0.600	-2105.6
DUP			
C6H1102r_20+HO2=C6H12O4_Olef_18	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_4	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_4	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_2	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_2	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_4	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_4	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_2	3.35E10	0.600	-2105.6
DUP			
C6H1102r_4(m3)+HO2=C6H12O4_Olef_2	3.35E10	0.600	-2105.6
DUP			
C*CC*CCOOH=>C5H7Or_Olef_1+OH	1.59E20	-1.500	42857.5
C*CC(OOH)C*C=>C5H7Or_Olef_3+OH	1.59E20	-1.500	42857.5
C5H8O3_Olef_1=>C5H7O2r_Olef_1+OH	1.59E20	-1.500	42857.5
C5H8O3_Olef_3=>C5H7O2r_Olef_3+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_4=>C6H9O2r_Olef(m4)+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_10=>C6H9O2r_Olef_10+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_12=>C6H9O2r_Olef_12+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_15=>C6H9O2r_Olef_14+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_17=>C6H9O2r_Olef_17+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_18=>C6H9O2r_Olef(m1)+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_2=>C6H9O2r_Olef_2+OH	1.59E20	-1.500	42857.5
C6H1003_Olef_7=>C6H9O2r_Olef_7+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_4=>C6H11O3r_5(m0)+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_4=>C6H11O3r_7(m5)+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_15=>C6H11O3r_28+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_15=>C6H11O3r_19+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_12=>C6H11O3r_23+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_12=>C6H11O3r_20+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_18=>C6H11O3r_32+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_18=>C6H11O3r_38+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_20=>C6H11O3r_46+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_20=>C6H11O3r_47+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_23=>C6H11O3r_40+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_23=>C6H11O3r_43+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_2=>C6H11O3r_10+OH	1.59E20	-1.500	42857.5
C6H12O4_Olef_2=>C6H11O3r_13+OH	1.59E20	-1.500	42857.5

C5H7O2r_Olef_3=C2H3CHO+CH2CHO	3.00E13	0.220	14098.6
C6H11O3r_13=CH3+C5H8O3_Olef_1	9.00E13	0.220	14098.6
C6H11O3r_13=CH3CHO+C4H7O2r_Olef	9.00E13	0.220	14098.6
C6H11O3r_5(m0)=C4H7O2r_Olef_1+CH3CHO	9.00E13	0.220	14098.6
C6H11O3r_5(m0)=C5H8O3_Olef_3+CH3	9.00E13	0.220	14098.6
C6H11O3r_19=C2H5+C4H6O3_Olef	9.00E13	0.220	14098.6
C6H11O3r_20=C2H3CHO+C3H7O2r_2	9.00E13	0.220	14098.6
C6H11O3r_23=C2H5+C4H6O3_Olef_3	9.00E13	0.220	14098.6
C6H11O3r_23=C2H5CHO+C3H5O2r_Olef_1	9.00E13	0.220	14098.6
C6H11O3r_32=C5H9O2r_Olef_4+CH2O	9.00E13	0.220	14098.6
C6H11O3r_38=C5H8O_Olef_1+CH2O2H	9.00E13	0.220	14098.6
C6H11O3r_43=C5H9O2r_Olef_5+CH2O	3.00E13	0.220	14098.6
C6H11O3r_46=C5H9O2r_Olef_8+CH2O	3.00E13	0.220	14098.6
C6H11O3r_47=C2H3CHO+C3H6OOH1-3	3.00E13	0.220	14098.6
C6H11O3r_7(m5)=C2H3CHO+C3H6OOH1-2	9.00E13	0.220	14098.6
C6H9O2r_Olef(m4)=CH3+C5H6O2_Olef_1	9.00E13	0.220	14098.6
C6H9O2r_Olef(m4)=CH3CHO+C*CCJC*O	9.00E13	0.220	14098.6
C6H9O2r_Olef_10=C4H4O2_Olef_2+C2H5	9.00E13	0.220	14098.6
C6H9O2r_Olef_12=C2H5+C4H4O2_Olef_1	9.00E13	0.220	14098.6
C6H9O2r_Olef_17=C5H7Or_Olef_4+CH2O	3.00E13	0.220	14098.6
C6H9O2r_Olef(m1)=C5H7Or_Olef_6+CH2O	3.00E13	0.220	14098.6
C6H9O2r_Olef_2=C4H5Or_Olef_1+CH3CHO	9.00E13	0.220	14098.6
C6H9O2r_Olef_2=C5H6O2_Olef_2+CH3	9.00E13	0.220	14098.6
C5H7O2r_Olef_1=C5H6O2_Olef_1+H	1.17E10	1.000	18548.8
C5H7O2r_Olef_3=C5H6O2_Olef_2+H	5.87E9	1.000	18548.8
C5H7Or_Olef_1=C5H6O_Olef_1+H	1.17E10	1.000	18548.8
C5H7Or_Olef_3=C5H6O_Olef_2+H	1.17E10	1.000	18548.8
C6H11O3r_10=C6H10O3_Olef_4+H	3.52E10	1.000	18548.8
C6H11O3r_28=C6H10O3_Olef_12+H	3.52E10	1.000	18548.8
C6H11O3r_19=C6H10O3_Olef_7+H	1.76E10	1.000	18548.8
C6H11O3r_20=C6H10O3_Olef_10+H	1.76E10	1.000	18548.8
C6H11O3r_38=C6H10O3_Olef_15+H	1.76E10	1.000	18548.8
C6H11O3r_40=C6H10O3_Olef_17+H	1.17E10	1.000	18548.8
C6H11O3r_47=C6H10O3_Olef_18+H	5.87E9	1.000	18548.8
C6H11O3r_7(m5)=C6H10O3_Olef_2+H	1.76E10	1.000	18548.8
C6H9O2r_Olef_12=C6H8O2_Olef_1+H	1.76E10	1.000	18548.8
C6H9O2r_Olef_7=C6H8O2_Olef_1+H	3.52E10	1.000	18548.8
C5H7O2r_Olef_1=C4H5Or_Olef+CH2O	2.70E14	0.000	23890.4
C5H7O2r_Olef_3=C2H3+C3H4O2	2.70E14	0.000	23890.4
C5H7Or_Olef_1=C4H5-N+CH2O	2.70E14	0.000	23890.4
C5H7Or_Olef_3=C2H3+C2H3CHO	5.40E14	0.000	23890.4
C6H11O3r_10=C5H9O2r_Olef_1+CH2O	8.10E14	0.000	23890.4
C6H11O3r_28=C5H9O2r_Olef_2+CH2O	8.10E14	0.000	23890.4
C6H11O3r_19=C2H5CHO+C3H5O2r_Olef	8.10E14	0.000	23890.4
C6H11O3r_20=C2H3+NC4KET12	8.10E14	0.000	23890.4
C6H11O3r_38=C4H71-1+C2H4O3	8.10E14	0.000	23890.4
C6H11O3r_40=C5H9O2r_Olef_7+CH2O	2.70E14	0.000	23890.4
C6H11O3r_47=C2H3+NC4KET14	2.70E14	0.000	23890.4
C6H11O3r_7(m5)=C2H3+NC4KET13	8.10E14	0.000	23890.4
C6H9O2r_Olef_12=C2H5CHO+CJ*CC*O	8.10E14	0.000	23890.4
C6H9O2r_Olef_7=C5H7Or_Olef(m6)+CH2O	8.10E14	0.000	23890.4
O2+C*CCCCCJ=C*CCCCOOJ	5.20E11	0.230	-1579.8
O2+C6H11=C6H11O2r_1(m2)	3.02E15	-0.920	-129.1
DUP			
O2+C6H11=C6H11O2r_1(m2)	3.02E15	-0.920	-129.1
DUP			
O2+C6H11r_Olef=C6H11O2r_9	3.02E15	-0.920	-129.1
DUP			

O2+C6H11r_Olef=C6H11O2r_9 3.02E15 -0.920 -129.1
DUP
O2+C*CCJCCC=C6H11O2r_16 2.90E7 1.590 1080.3
DUP
O2+C*CCJCCC=C6H11O2r_16 2.90E7 1.590 1080.3
DUP
O2+C*CCJCCC=C6H11O2r_18 2.90E7 1.590 1080.3
DUP
O2+C*CCJCCC=C6H11O2r_18 2.90E7 1.590 1080.3
DUP
C6H11O2r_1(m2)=C6H11O2r_1 7.68E12 -0.130 34358.6
C*CCCCOOJ=C*CCCCJCP 4.66E7 1.400 28658.5
C6H11O2r_1(m2)=C6H11O2r_3 4.66E7 1.400 28658.5
C6H11O2r_16=C6H11O2r_24 4.66E7 1.400 28658.5
C6H11O2r_9=C6H11O2r_13 4.66E7 1.400 28658.5
C6H11O2r_9=C6H11O2r_14 9.82E0 2.655 18214.2
C6H11O2r_9=C6H11O2r_15 1.76E9 0.780 21849.4
C*CCCCOOJ=C*CCCJCCP 1.64E11 0.130 19468.9
C6H11O2r_16=C6H11O2r_22 1.64E11 0.130 19468.9
C6H11O2r_1(m2)=C6H11O2r_4(m3) 1.12E5 2.010 12124.5
C6H11O2r_16=C6H11O2r_23 6.18E7 1.000 21070.2
C6H11O2r_18=C6H11O2r_20 8.94E6 1.290 14239.6
C*CCCCOOJ=C*CCJCCCP 2.58E7 0.960 14289.8
C6H11O2r_1(m2)=C6H10+HO2 8.66E9 0.930 29799.3
C*CCCCOOJ=C6H10+HO2 5.77E9 0.930 29799.3
C6H11O2r_1(m2)=C6H10_Olef_3+HO2 5.77E9 0.930 29799.3
C6H11O2r_16=C6H10_Olef_1+HO2 5.77E9 0.930 29799.3
C6H11O2r_9=C6H10_Olef_3+HO2 5.77E9 0.930 29799.3
C6H11O2r_9=C6H10_Olef_1+HO2 3.16E10 0.637 27578.2
C*CCCCJCP=C3H5-A+AC3H5OOH 9.15E12 0.000 20554.0
C*CCCJCCP=C*CCC*C+CH2O2H 6.65E13 0.000 26935.3
C*CCJCCCP=C4H6+C2H4O2H 1.72E14 0.000 37379.6
C6H11O2r_13=C3H5-A+C3H6O2_Olef_1 9.78E12 0.000 19526.3
C6H11O2r_14=C4H6O2_Olef_1+C2H5 1.83E14 0.000 36351.9
C6H11O2r_15=C4H7O2r_Olef_3+C2H4 1.71E14 0.000 25118.9
C6H11O2r_20=CH3+C*CC*CCOOH 2.39E14 0.000 39458.9
C6H11O2r_24=CH3+C*CC(OOH)*C4 2.27E13 0.000 30520.3
C6H11O2r_22=C3H6+C3H5O2r_Olef_1 4.27E13 0.000 30520.3
C6H11O2r_23=C2H4+C4H7O2r_Olef_1 5.05E13 0.000 28632.2
C6H11O2r_1=C4H71-4+C2H3OOH 5.40E13 0.000 27604.5
C6H11O2r_3=C5H8O2_Olef+CH3 4.57E13 0.000 29492.6
C6H11O2r_4(m3)=C4H6+C2H5O2r 5.80E14 0.000 33866.3
C6H11O2r_13=C6H10_Olef_3+HO2 1.83E10 0.790 15099.6
C6H11O2r_14=C6H10_Olef_1+HO2 1.83E10 0.790 15099.6
C6H11O2r_20=C6H10_Olef_1+HO2 1.83E10 0.790 15099.6
C6H11O2r_24=C6H10_Olef_1+HO2 1.83E10 0.790 15099.6
C6H11O2r_3=C6H10_Olef_3+HO2 1.83E10 0.790 15099.6
C6H11O2r_13=C6H10O_Olef_3+OH 2.28E8 1.290 9889.8
C6H11O2r_14=C6H10O_Olef_12+OH 2.28E8 1.290 9889.8
C6H11O2r_20=C6H10O_Olef_22+OH 2.28E8 1.290 9889.8
C6H11O2r_24=C6H10O_Olef_12+OH 2.28E8 1.290 9889.8
C6H11O2r_3=C6H10O_Olef_3+OH 2.28E8 1.290 9889.8
C*CCCJCCP=C6H10O_Olef_14+OH 4.58E15 -1.080 18438.9
C6H11O2r_15=C6H10O_Olef_14+OH 9.16E15 -1.080 18438.9
C6H11O2r_22=C6H10O_Olef_(m7)+OH 4.58E15 -1.080 18438.9
!C6H11O2r_4(m3)=C6H10O_Olef_(m7)+OH 4.58E15 -1.080 18438.9 !
RDB
C*CCJCCCP=C6H10O_Olef_25+OH 3.50E10 0.100 9330.6

C6H11O2r_23=C6H10O_olef_25+OH	7.00E10	0.100	9330.6	
C6H11O2r_14=C6H10O_olef_17+OH	3.50E10	0.100	9330.6	
C6H11O2r_20=C6H10O_olef_17+OH	3.50E10	0.100	9330.6	
C*CC*CCJ+HO2=C*CC*CCOOH	6.70E10	0.600	-2105.6	
DUP				
C*CC*CCJ+HO2=C*CC*CCOOH	6.70E10	0.600	-2105.6	
DUP				
C*CC*CCJ+HO2=C*CC(OOH)C*C	6.70E10	0.600	-2105.6	
Ccy(CJC*CC*C)+CH3=Ccy(C(C)C*CC*C)		8.34E14	-0.700	-
500.0				
Ccy(CJC*CC*C)+CH3=Ccy(CC(C)*CC*C)		8.34E14	-0.700	-
500.0				
Ccy(CJC*CC*C)+CH3=Ccy(CC*C(C)C*C)		8.34E14	-0.700	-
500.0				
Ccy(CC(C)*CC*C)=Ccy(C*C(C)C*CC)		7.04E8	1.200	
24808.2				
Ccy(CC*C(C)C*C)=Ccy(C*CC(C)*CC)		7.04E8	1.200	
24808.2				
Ccy(CC*C(C)C*C)=Ccy(C*CC*C(C)C)		7.04E8	1.200	
24808.2				
Ccy(C*C(C)C*CC)=Ccy(C*CCC*C(C))		2.21E7	2.100	
25095.0				
C*CCcyCJC*CC*C=C*CCJcyCC*CC*C		1.47E-3	4.910	
40391.0				
C*CCJcyCC*CC*C=C*CC*cycCJC*CC		1.10E7	1.540	
13407.9				
C*CC*cycCJC*CC=C*CC*cycCJCC*C		9.20E3	2.810	
30209.6				
C*CCJcyCC*CC*C=bicyclicC8H9	1.60E11	0.170	4397.6	
bicyclicC8H9=C*CCcyCC*CC*CCJ	8.50E11	0.410	16706.1	
C*CCcyCC*CC*CCJ=C6H5C2H3+H	9.00E8	1.300	27389.4	
C*CCcyCC*CC*C=C*CCcy(C*CC*CC)		7.04E8	1.200	
24808.2				
C*CCcy(C*CC*CC)=C*CCcy(C*CCC*C)		5.52E6	2.100	
25095.0				
C2H3+C*CCcy(C*CC*CC)=C2H4+C*CC*cycCJC*CC		1.73E13	0.000	
5114.6				
C2H3+C*CCcy(C*CC*CC)=C2H4+C*CCcyCJC*CC*C		1.70E13	0.000	
15367.7				
C2H3+C*CCcy(C*CCC*C)=C2H4+C*CC*cycCJCC*C		1.73E13	0.000	
5114.6				
C2H3+C*CCcy(C*CCC*C)=C2H4+C*CCcyCJC*CC*C		1.70E13	0.000	
15367.7				
C2H3+C*CCcyCC*CC*C=C2H4+C*CCJcyCC*CC*C		1.61E13	0.000	
7361.2				
C2H3+C*CCcyCC*CC*C=C2H4+C*CCcyCJC*CC*C		8.52E12	0.000	
15367.7				
C2H5+C*CCcy(C*CC*CC)=C2H6+C*CC*cycCJC*CC		2.89E12	0.000	
11209.1				
C2H5+C*CCcy(C*CC*CC)=C2H6+C*CCcyCJC*CC*C		2.85E12	0.000	
21462.2				
C2H5+C*CCcy(C*CCC*C)=C2H6+C*CC*cycCJCC*C		2.89E12	0.000	
11209.1				
C2H5+C*CCcy(C*CCC*C)=C2H6+C*CCcyCJC*CC*C		2.85E12	0.000	
21462.2				
C2H5+C*CCcyCC*CC*C=C2H6+C*CCJcyCC*CC*C		2.69E12	0.000	
13455.7				

C2H5+C*CCcyCC*CC*C=C2H6+C*CCcyCJC*CC*C 21462.2	1.42E12	0.000	
C3H5-A+C*CCcy(C*CC*CC)=C3H6+C*CC*cyCCJC*CC 24179.2	3.85E13	0.000	
C3H5-A+C*CCcy(C*CCC*C)=C3H6+C*CC*cyCCJCC*C 24179.2	3.85E13	0.000	
C3H5-A+C*CCcyCC*CC*C=C3H6+C*CCJcyCC*CC*C 24425.8	3.58E13	0.000	
CH3+C*CCcy(C*CC*CC)=CH4+C*CC*cyCCJC*CC 9918.5	1.78E13	0.000	
CH3+C*CCcy(C*CCC*C)=CH4+C*CC*cyCCJCC*C 9918.5	1.78E13	0.000	
CH3+C*CCcyCC*CC*C=CH4+C*CCJcyCC*CC*C 12165.1	1.66E13	0.000	
H+C*CCcy(C*CC*CC)=H2+C*CC*cyCCJC*CC 6190.1	2.01E14	0.000	
H+C*CCcy(C*CC*CC)=H2+C*CCcyCJC*CC*C 6190.1	2.01E14	0.000	
H+C*CCcy(C*CCC*C)=H2+C*CC*cyCCJCC*C 6190.1	2.01E14	0.000	
H+C*CCcy(C*CCC*C)=H2+C*CCcyCJC*CC*C 6190.1	2.01E14	0.000	
H+C*CCcyCC*CC*C=H2+C*CCJcyCC*CC*C 7170.0	1.52E14	0.000	
H+C*CCcyCC*CC*C=H2+C*CCcyCJC*CC*C 5114.6	4.39E13	0.000	
OH+C*CCcy(C*CC*CC)=H2O+C*CC*cyCCJC*CC -1362.3	5.20E5	2.300	
OH+C*CCcy(C*CC*CC)=H2O+C*CCcyCJC*CC*C -1362.3	5.20E5	2.300	
OH+C*CCcy(C*CCC*C)=H2O+C*CC*cyCCJCC*C -1362.3	5.20E5	2.300	
OH+C*CCcy(C*CCC*C)=H2O+C*CCcyCJC*CC*C -1362.3	5.20E5	2.300	
OH+C*CCcyCC*CC*C=H2O+C*CCJcyCC*CC*C -1362.3	5.20E5	2.300	
OH+C*CCcyCC*CC*C=H2O+C*CCcyCJC*CC*C -1362.3	2.60E5	2.300	
H02+C*CCcy(C*CC*CC)=H2O2+C*CC*cyCCJC*CC 13546.5	5.12E-2	4.400	
H02+C*CCcy(C*CC*CC)=H2O2+C*CCcyCJC*CC*C 13546.5	5.12E-2	4.400	
H02+C*CCcy(C*CCC*C)=H2O2+C*CC*cyCCJCC*C 13546.5	5.12E-2	4.400	
H02+C*CCcy(C*CCC*C)=H2O2+C*CCcyCJC*CC*C 13546.5	5.12E-2	4.400	
H02+C*CCcyCC*CC*C=H2O2+C*CCJcyCC*CC*C 13546.5	5.12E-2	4.400	
H02+C*CCcyCC*CC*C=H2O2+C*CCcyCJC*CC*C 13546.5	2.56E-2	4.400	
CCcyCJC*CC*C=CCJcyCC*CC*C	1.47E-3	4.910	40391.0
CCJcyCC*CC*C=CC*cy(CCJC*CC)	1.10E7	1.540	13407.9
CC*cy(CCJC*CC)=CC*cy(CCJCC*C) 30209.6	2.30E3	2.810	
CCJcyCC*CC*C=bicyclic7H9	1.60E11	0.170	4397.6
bicyclic7H9=Ccy(CCJC*CC*C)	8.50E11	0.410	16706.1
CCcyCC*CC*C=CCcyC*CC*CC	7.04E8	1.200	24808.2
CCcyC*CC*CC=CCcyC*CCC*C	1.66E7	2.100	25095.0

C*CC*cyCC*CC*C+H=C*CCcyCJC*CC*C 700.3	1.70E9	1.460	-
C*CC*cyCC*CC*C+H=C*CCJcyCC*CC*C 2000.4	6.50E7	1.760	
C*CC*cyCC*CC*C+H=C*CC*cyCCJCC*C	1.75E9	1.520	901.0
C*CC*cyCC*CC*C+H=C*CC*cyCCJC*CC	3.66E9	1.480	399.1
C10H10=C10H10_2	1.41E9	1.200	24808.2
C10H10_2=C10H10_1	7.04E8	1.200	24808.2
C10H10_3=C10H10_5	7.04E8	1.200	24808.2
C10H10_2=C10H10_3	5.52E6	2.100	25095.0
C10H10_5=C10H10_1	5.52E6	2.100	25095.0
C10H10_5=C10H10_4	5.52E6	2.100	25095.0
C2H3+C10H10=C2H4+CPDcyCJC*CC*C 15367.7	1.70E13	0.000	
C2H3+C10H10_1=C2H4+CPD*cyCC*CCJC 15367.7	3.41E13	0.000	
C2H3+C10H10_2=C2H4+CPD*cyCC*CCJC 15367.7	8.52E12	0.000	
C2H3+C10H10_2=C2H4+CPDcyCJC*CC*C 15367.7	1.70E13	0.000	
C2H3+C10H10_3=C2H4+CPD*cyCC*CCCJ 15367.7	8.52E12	0.000	
C2H3+C10H10_3=C2H4+CPDcyCJC*CC*C 15367.7	1.70E13	0.000	
C2H3+C10H10_4=C2H4+CPD*cyCC*CCCJ 15367.7	3.41E13	0.000	
C2H3+C10H10_5=C2H4+CPD*cyCC*CCCJ 15367.7	1.70E13	0.000	
C2H3+C10H10_5=C2H4+CPD*cyCC*CCJC 15367.7	1.70E13	0.000	
C2H5+C10H10=C2H6+CPDcyCJC*CC*C 21462.2	2.85E12	0.000	
C2H5+C10H10_1=C2H6+CPD*cyCC*CCJC 21462.2	5.69E12	0.000	
C2H5+C10H10_2=C2H6+CPD*cyCC*CCJC 21462.2	1.42E12	0.000	
C2H5+C10H10_2=C2H6+CPDcyCJC*CC*C 21462.2	2.85E12	0.000	
C2H5+C10H10_3=C2H6+CPD*cyCC*CCCJ 21462.2	1.42E12	0.000	
C2H5+C10H10_3=C2H6+CPDcyCJC*CC*C 21462.2	2.85E12	0.000	
C2H5+C10H10_4=C2H6+CPD*cyCC*CCCJ 21462.2	5.69E12	0.000	
C2H5+C10H10_5=C2H6+CPD*cyCC*CCCJ 21462.2	2.85E12	0.000	
C2H5+C10H10_5=C2H6+CPD*cyCC*CCJC 21462.2	2.85E12	0.000	
C3H3+C10H10=C3H4-A+CPDcyCJC*CC*C 28751.7	1.01E13	0.000	
C3H3+C10H10=C3H4-P+CPDcyCJC*CC*C 28751.7	1.01E13	0.000	
C3H3+C10H10_1=C3H4-A+CPD*cyCC*CCJC 28751.7	2.01E13	0.000	
C3H3+C10H10_1=C3H4-P+CPD*cyCC*CCJC 28751.7	2.01E13	0.000	
C3H3+C10H10_2=C3H4-A+CPD*cyCC*CCJC 28751.7	5.03E12	0.000	

C3H3+C10H10_2=C3H4-A+CPDcyCJC*CC*C 28751.7	1.01E13	0.000
C3H3+C10H10_2=C3H4-P+CPD*cyCC*CCJC 28751.7	5.03E12	0.000
C3H3+C10H10_2=C3H4-P+CPDcyCJC*CC*C 28751.7	1.01E13	0.000
C3H3+C10H10_3=C3H4-A+CPD*cyCC*CCCJ 28751.7	5.03E12	0.000
C3H3+C10H10_3=C3H4-A+CPDcyCJC*CC*C 28751.7	1.01E13	0.000
C3H3+C10H10_3=C3H4-P+CPD*cyCC*CCCJ 28751.7	5.03E12	0.000
C3H3+C10H10_3=C3H4-P+CPDcyCJC*CC*C 28751.7	1.01E13	0.000
C3H3+C10H10_4=C3H4-A+CPD*cyCC*CCCJ 28751.7	2.01E13	0.000
C3H3+C10H10_4=C3H4-P+CPD*cyCC*CCCJ 28751.7	2.01E13	0.000
C3H3+C10H10_5=C3H4-A+CPD*cyCC*CCCJ 28751.7	1.01E13	0.000
C3H3+C10H10_5=C3H4-A+CPD*cyCC*CCJC 28751.7	1.01E13	0.000
C3H3+C10H10_5=C3H4-P+CPD*cyCC*CCCJ 28751.7	1.01E13	0.000
C3H3+C10H10_5=C3H4-P+CPD*cyCC*CCJC 28751.7	1.01E13	0.000
!C3H5-A+C10H10=C3H6+CPDcyCJC*CC*C 32432.3	3.79E13	0.000
!C3H5-A+C10H10_1=C3H6+CPD*cyCC*CCJC 32432.3	7.58E13	0.000
!C3H5-A+C10H10_2=C3H6+CPD*cyCC*CCJC 32432.3	1.89E13	0.000
!C3H5-A+C10H10_2=C3H6+CPDcyCJC*CC*C 32432.3	3.79E13	0.000
!C3H5-A+C10H10_3=C3H6+CPD*cyCC*CCCJ 32432.3	1.89E13	0.000
!C3H5-A+C10H10_3=C3H6+CPDcyCJC*CC*C 32432.3	3.79E13	0.000
!C3H5-A+C10H10_4=C3H6+CPD*cyCC*CCCJ 32432.3	7.58E13	0.000
!C3H5-A+C10H10_5=C3H6+CPD*cyCC*CCCJ 32432.3	3.79E13	0.000
!C3H5-A+C10H10_5=C3H6+CPD*cyCC*CCJC 32432.3	3.79E13	0.000
C3H5-S+C10H10=C3H6+CPDcyCJC*CC*C 15367.7	1.70E13	0.000
C3H5-S+C10H10_1=C3H6+CPD*cyCC*CCJC 15367.7	3.41E13	0.000
C3H5-S+C10H10_2=C3H6+CPD*cyCC*CCJC 15367.7	8.52E12	0.000
C3H5-S+C10H10_2=C3H6+CPDcyCJC*CC*C 15367.7	1.70E13	0.000
C3H5-S+C10H10_3=C3H6+CPD*cyCC*CCCJ 15367.7	8.52E12	0.000
C3H5-S+C10H10_3=C3H6+CPDcyCJC*CC*C 15367.7	1.70E13	0.000
C3H5-S+C10H10_4=C3H6+CPD*cyCC*CCCJ 15367.7	3.41E13	0.000

C3H5-S+C10H10_5=C3H6+CPD*cyCC*CCCJ 15367.7	1.70E13	0.000	
C3H5-S+C10H10_5=C3H6+CPD*cyCC*CCJC 15367.7	1.70E13	0.000	
C3H5-T+C10H10=C3H6+CPDcyCJC*CC*C 16371.5	1.26E13	0.000	
C3H5-T+C10H10_1=C3H6+CPD*cyCC*CCJC 16371.5	2.53E13	0.000	
C3H5-T+C10H10_2=C3H6+CPD*cyCC*CCJC 16371.5	6.31E12	0.000	
C3H5-T+C10H10_2=C3H6+CPDcyCJC*CC*C 16371.5	1.26E13	0.000	
C3H5-T+C10H10_3=C3H6+CPD*cyCC*CCCJ 16371.5	6.31E12	0.000	
C3H5-T+C10H10_3=C3H6+CPDcyCJC*CC*C 16371.5	1.26E13	0.000	
C3H5-T+C10H10_4=C3H6+CPD*cyCC*CCCJ 16371.5	2.53E13	0.000	
C3H5-T+C10H10_5=C3H6+CPD*cyCC*CCCJ 16371.5	1.26E13	0.000	
C3H5-T+C10H10_5=C3H6+CPD*cyCC*CCJC 16371.5	1.26E13	0.000	
!CH3+C10H10=CH4+CPDcyCJC*CC*C 20171.6	1.76E13	0.000	
!CH3+C10H10_1=CH4+CPD*cyCC*CCJC 20171.6	3.51E13	0.000	
!CH3+C10H10_2=CH4+CPD*cyCC*CCJC 20171.6	8.78E12	0.000	
!CH3+C10H10_2=CH4+CPDcyCJC*CC*C 20171.6	1.76E13	0.000	
!CH3+C10H10_3=CH4+CPD*cyCC*CCCJ 20171.6	8.78E12	0.000	
!CH3+C10H10_3=CH4+CPDcyCJC*CC*C 20171.6	1.76E13	0.000	
!CH3+C10H10_4=CH4+CPD*cyCC*CCCJ 20171.6	3.51E13	0.000	
!CH3+C10H10_5=CH4+CPD*cyCC*CCCJ 20171.6	1.76E13	0.000	
!CH3+C10H10_5=CH4+CPD*cyCC*CCJC 20171.6	1.76E13	0.000	
!H+C10H10=H2+CPDcyCJC*CC*C	1.03E14	0.000	5210.2
!H+C10H10_1=H2+CPD*cyCC*CCJC	4.03E14	0.000	6190.1
!H+C10H10_2=H2+CPD*cyCC*CCJC	3.19E14	0.000	15869.6
!H+C10H10_2=H2+CPDcyCJC*CC*C	2.01E14	0.000	6190.1
!H+C10H10_3=H2+CPD*cyCC*CCCJ	3.19E14	0.000	15869.6
!H+C10H10_3=H2+CPDcyCJC*CC*C	2.01E14	0.000	6190.1
!H+C10H10_4=H2+CPD*cyCC*CCCJ	4.03E14	0.000	6190.1
!H+C10H10_5=H2+CPD*cyCC*CCCJ	2.01E14	0.000	6190.1
!H+C10H10_5=H2+CPD*cyCC*CCJC	2.01E14	0.000	6190.1
OH+C10H10=H2O+CPDcyCJC*CC*C	5.20E5	2.300	-1362.3
OH+C10H10_1=H2O+CPD*cyCC*CCJC 1362.3	1.04E6	2.300	-
OH+C10H10_2=H2O+CPD*cyCC*CCJC 1362.3	2.60E5	2.300	-
OH+C10H10_2=H2O+CPDcyCJC*CC*C 1362.3	5.20E5	2.300	-
OH+C10H10_3=H2O+CPD*cyCC*CCCJ 1362.3	2.60E5	2.300	-

OH+C10H10_3=H2O+CPDcyCJC*CC*C 1362.3	5.20E5	2.300	-
OH+C10H10_4=H2O+CPD*cyCC*CCCJ 1362.3	1.04E6	2.300	-
OH+C10H10_5=H2O+CPD*cyCC*CCCJ 1362.3	5.20E5	2.300	-
OH+C10H10_5=H2O+CPD*cyCC*CCJC 1362.3	5.20E5	2.300	-
HO2+C10H10=H2O2+CPDcyCJC*CC*C 13546.5	5.12E-2	4.400	
HO2+C10H10_1=H2O2+CPD*cyCC*CCJC 13546.5	1.02E-1	4.400	
HO2+C10H10_2=H2O2+CPD*cyCC*CCJC 13546.5	2.56E-2	4.400	
HO2+C10H10_2=H2O2+CPDcyCJC*CC*C 13546.5	5.12E-2	4.400	
HO2+C10H10_3=H2O2+CPD*cyCC*CCCJ 13546.5	2.56E-2	4.400	
HO2+C10H10_3=H2O2+CPDcyCJC*CC*C 13546.5	5.12E-2	4.400	
HO2+C10H10_4=H2O2+CPD*cyCC*CCCJ 13546.5	1.02E-1	4.400	
HO2+C10H10_5=H2O2+CPD*cyCC*CCCJ 13546.5	5.12E-2	4.400	
HO2+C10H10_5=H2O2+CPD*cyCC*CCJC 13546.5	5.12E-2	4.400	
C3H5-A+C3H4-A=C3H6+C3H3	9.87E+13	0.000	32432.3
C3H5-A+C3H4-P=C3H6+C3H3	5.27E+13	0.000	26815.8
C3H5-A+C3H6=C3H6+C3H5-S	1.89E+13	0.000	32432.3
C3H5-A+C3H6=C3H6+C3H5-T	2.12E+13	0.000	30233.5
C*CJCCC*C=C6H9r_R5_7	3.74E10	0.000	14363.9
CJ*CCCC*C=Cy(C*CCCJCC)	5.22E9	0.000	7217.8
CJ*CCCC*C=CJcy(CC*CCC)	1.40E10	0.000	6649.9
C6H11=CJcy(CCCC)C	1.35E+06	1.48	12200 ! RDB changed to Kun -
original 1.00E11 0.000 17481.2			
C*CC(C)CCJ=CJcy(CCCC)C	1.35E+06	1.48	12200 ! RDB changed to Kun -
original 2.00E11 0.000 18604.5			
C*CC(C)CCJ=C4H71-3+C2H4	1.23E13	0.000	19311.2
C*CC(C)CCJ=Ccy(CCJCCC)	7.25E+07	0.83	14100 ! RDB changed to Kun -
original 7.48E10 0.000 17662.1			
C*C*CcyCC*CC*C+H=C*CCJcyCC*CC*C 6476.9	5.50E13	0.000	
DUP			
C*C*CcyCC*CC*C+H=C*CCJcyCC*CC*C 5903.3	5.74E13	0.000	
DUP			
C*CcyCC*CC*C+H=CCJcyCC*CC*C	5.56E13	0.000	3847.9
C*CcyCC*CC*C+H=CJcycyCC*CC*C	6.46E13	0.000	5377.5
C*cy(CC*CC*CC)+H=C*cy(CC*CCCJC) 5377.5	8.20E13	0.000	
C*cy(CC*CC*CC)+H=C*cy(CCC*CCJC) 4278.1	7.43E13	0.000	
C*cy(CC*CC*CC)+H=CJcy(C*CC*CCC) 3704.5	6.11E13	0.000	
C*cy(CC*CC*CC)+H=CJcy(C*CCC*CC) 4278.1	7.43E13	0.000	
C*cy(CC*CC*CC)+H=CJcy(CC*CC*CC) 6739.8	2.53E13	0.000	

C*cy (CC*CC*CC) +H=Ccy (CJCC*CC*C) 2294.4	5.61E13	0.000	
C*cy (CC*CCC*C) +H=C*cy (CC*CCCJC) 5377.5	1.64E14	0.000	
C*cy (CC*CCC*C) +H=C7H9r_Olef	1.22E14	0.000	3704.5
C*cy (CC*CCC*C) +H=C7H9r_Olef_1 7456.8	6.78E13	0.000	
C*cy (CC*CCC*C) +H=Ccy (C*CCJCC*C) 1696.9	1.01E14	0.000	
C*C*CCCJC*C=CJcy (C*CCC*CC)	5.22E9	0.000	19574.1
CJcy (C*CC*CCC) =Ccy (C*CCCJC*C) 48517.0	2.40E12	0.000	
CJcy (C*CCC*CC) =Ccy (C*CCCJC*C) 56523.5	2.40E12	0.000	
CJcy (CC*CC*CC) =Ccy (CCJC*CC*C) 37546.9	4.80E12	0.000	
C4H6+C3H3=C*C*CCCJC*C	3.19E12	0.000	3585.0
CH3+C*cy (CC*CC*CC) =CH4+C7H7	1.76E13	0.000	20171.6
CH3+C*cy (CC*CCC*C) =CH4+C7H7	1.76E13	0.000	20171.6
H+C*cy (CC*CC*CC) =H2+C7H7	2.01E14	0.000	6190.1
H+C*cy (CC*CCC*C) =H2+C7H7	2.01E14	0.000	6190.1
OH+C*cy (CC*CC*CC) =H2O+C7H7	5.20E5	2.300	-1362.3
OH+C*cy (CC*CCC*C) =H2O+C7H7	5.20E5	2.300	-1362.3
HO2+C*cy (CC*CC*CC) =H2O2+C7H7	5.12E-2	4.400	13546.5
HO2+C*cy (CC*CCC*C) =H2O2+C7H7	5.12E-2	4.400	13546.5
C2H3+Ccy (CCC*CCC) =C2H4+CJcy (CCC*CCC)	2.31E13	0.000	12451.9
C2H3+Ccy (CCC*CCC) =C2H4+Ccy (CCC*CCJC)	1.20E13	0.000	6142.3
C2H3+Ccy (CCC*CCC) =C2H4+Ccy (CCJCC*CC)	1.65E13	0.000	10157.5
C2H3+Ccy (CCC*CCC) =C2H4+Ccy (CCJC*CCC)	1.21E13	0.000	6142.3
C2H3+Ccy (CCC*CCC) =C2H4+Ccy (CJCC*CCC)	9.99E12	0.000	7982.6
C2H3+Ccy (CC*CCCC) =C2H4+Ccy (CCJC*CCC)	1.20E13	0.000	6142.3
C2H3+Ccy (CC*CCCC) =C2H4+CJcy (CC*CCCC)	3.01E13	0.000	12882.1
C2H3+Ccy (CC*CCCC) =C2H4+Ccy (CC*CCCJC)	1.64E13	0.000	10157.5
C2H3+Ccy (CC*CCCC) =C2H4+Ccy (CC*CCCCJ)	1.64E13	0.000	10157.5
C2H3+Ccy (CC*CCCC) =C2H4+Ccy (CJC*CCCC)	4.07E12	0.000	5473.1
C2H3+Ccy (C*CCCC) =C2H4+Ccy (C*CCCJCC)	1.64E13	0.000	10157.5
C2H3+Ccy (C*CCCC) =C2H4+Ccy (C*CCCCJC)	1.64E13	0.000	10157.5
C2H3+Ccy (C*CCCC) =C2H4+Ccy (C*CCCCCJ)	1.20E13	0.000	6142.3
C2H3+Ccy (C*CCCC) =C2H4+Ccy (CJC*CCCC)	1.20E13	0.000	6142.3
C2H3+Ccy (C*CCCC) =C2H4+CJcy (C*CCCC)	7.46E12	0.000	9034.2
C2H3+C*cy (CCCC) =C2H4+C*cy (CCCCJCC)	1.49E13	0.000	10133.6
C2H3+C*cy (CCCC) =C2H4+C*cy (CCCJCCC)	2.98E13	0.000	10133.6
C2H3+C*cy (CCCC) =C2H4+CJcy (C*CCCC)	2.98E13	0.000	10133.6
C2H5+Ccy (CCC*CCC) =C2H6+CJcy (CCC*CCC)	3.60E12	0.000	18546.4
C2H5+Ccy (CCC*CCC) =C2H6+Ccy (CCC*CCJC)	2.00E12	0.000	12236.8
C2H5+Ccy (CCC*CCC) =C2H6+Ccy (CCJCC*CC)	2.73E12	0.000	16252.0
C2H5+Ccy (CCC*CCC) =C2H6+Ccy (CCJC*CCC)	2.02E12	0.000	12236.8
C2H5+Ccy (CCC*CCC) =C2H6+Ccy (CJCC*CCC)	1.67E12	0.000	14077.1
C2H5+Ccy (CC*CCCC) =C2H6+Ccy (CCJC*CCC)	2.00E12	0.000	12236.8
C2H5+Ccy (CC*CCCC) =C2H6+CJcy (CC*CCCC)	4.71E12	0.000	18976.6
C2H5+Ccy (CC*CCCC) =C2H6+Ccy (CC*CCCJC)	2.70E12	0.000	16252.0
C2H5+Ccy (CC*CCCC) =C2H6+Ccy (CC*CCCCJ)	2.68E12	0.000	16252.0
C2H5+Ccy (CC*CCCC) =C2H6+Ccy (CJC*CCCC)	6.80E11	0.000	11567.6
C2H5+Ccy (C*CCCC) =C2H6+Ccy (C*CCCJCC)	2.70E12	0.000	16252.0
C2H5+Ccy (C*CCCC) =C2H6+Ccy (C*CCCCJC)	2.70E12	0.000	16252.0
C2H5+Ccy (C*CCCC) =C2H6+Ccy (C*CCCCCJ)	2.00E12	0.000	12236.8
C2H5+Ccy (C*CCCC) =C2H6+Ccy (CJC*CCCC)	2.00E12	0.000	12236.8
C2H5+Ccy (C*CCCC) =C2H6+CJcy (C*CCCC)	1.25E12	0.000	15128.7

C2H5+C*cy(CCCCCC)=C2H6+C*cy(CCCCJCC)	2.49E12	0.000	16228.1
C2H5+C*cy(CCCCCC)=C2H6+C*cy(CCCJCCC)	4.98E12	0.000	16228.1
C2H5+C*cy(CCCCCC)=C2H6+CJcy(C*CCCC)	4.98E12	0.000	16228.1
C3H5-A+Ccy(CCC*CCC)=C3H6+Ccy(CCC*CCJC)	2.66E13	0.000	23206.9
C3H5-A+Ccy(CCC*CCC)=C3H6+Ccy(CCJC*CCC)	2.68E13	0.000	23206.9
C3H5-A+Ccy(CCC*CCC)=C3H6+CJcy(CCC*CCC)	3.94E13	0.000	29516.5
C3H5-A+Ccy(CCC*CCC)=C3H6+Ccy(CCJCC*CC)	3.03E13	0.000	27222.1
C3H5-A+Ccy(CCC*CCC)=C3H6+Ccy(CJCC*CCC)	1.90E13	0.000	25047.2
C3H5-A+Ccy(C*CCCC)=C3H6+Ccy(C*CCCJCC)	3.00E13	0.000	27222.1
C3H5-A+Ccy(C*CCCC)=C3H6+Ccy(C*CCCCJC)	3.00E13	0.000	27222.1
C3H5-A+Ccy(C*CCCC)=C3H6+Ccy(C*CCCCCJ)	2.66E13	0.000	23206.9
C3H5-A+Ccy(C*CCCC)=C3H6+Ccy(CJC*CCCC)	2.66E13	0.000	23206.9
C3H5-A+Ccy(C*CCCC)=C3H6+CJcy(C*CCCC)	1.66E13	0.000	26098.8
C3H5-A+Ccy(CC*CCCC)=C3H6+CJcy(CC*CCCC)	5.17E13	0.000	29946.7
C3H5-A+Ccy(CC*CCCC)=C3H6+Ccy(CCJC*CCC)	2.66E13	0.000	23206.9
C3H5-A+Ccy(CC*CCCC)=C3H6+Ccy(CC*CCCJC)	2.99E13	0.000	27222.1
C3H5-A+Ccy(CC*CCCC)=C3H6+Ccy(CC*CCCCJ)	2.97E13	0.000	27222.1
C3H5-A+Ccy(CC*CCCC)=C3H6+Ccy(CJC*CCCC)	9.04E12	0.000	22537.7
C3H5-A+C*cy(CCCCCC)=C3H6+C*cy(CCCCJCC)	2.87E13	0.000	27198.2
C3H5-A+C*cy(CCCCCC)=C3H6+C*cy(CCCJCCC)	5.78E13	0.000	27198.2
C3H5-A+C*cy(CCCCCC)=C3H6+CJcy(C*CCCC)	6.63E13	0.000	27198.2
CH3+Ccy(CCC*CCC)=CH4+CJcy(CCC*CCC)	2.36E13	0.000	17255.8
CH3+Ccy(CCC*CCC)=CH4+Ccy(CCC*CCJC)	1.23E13	0.000	10946.2
CH3+Ccy(CCC*CCC)=CH4+Ccy(CCJCC*CC)	1.70E13	0.000	14961.4
CH3+Ccy(CCC*CCC)=CH4+Ccy(CCJC*CCC)	1.24E13	0.000	10946.2
CH3+Ccy(CCC*CCC)=CH4+Ccy(CJCC*CCC)	1.03E13	0.000	12786.5
CH3+Ccy(C*CCCC)=CH4+Ccy(C*CCCJCC)	1.69E13	0.000	14961.4
CH3+Ccy(C*CCCC)=CH4+Ccy(C*CCCCJC)	1.69E13	0.000	14961.4
CH3+Ccy(C*CCCC)=CH4+Ccy(C*CCCCCJ)	1.23E13	0.000	10946.2
CH3+Ccy(C*CCCC)=CH4+Ccy(CJC*CCCC)	1.23E13	0.000	10946.2
CH3+Ccy(C*CCCC)=CH4+CJcy(C*CCCC)	7.68E12	0.000	13838.1
CH3+Ccy(CC*CCCC)=CH4+CJcy(CC*CCCC)	3.09E13	0.000	17686.0
CH3+Ccy(CC*CCCC)=CH4+Ccy(CCJC*CCC)	1.23E13	0.000	10946.2
CH3+Ccy(CC*CCCC)=CH4+Ccy(CC*CCCJC)	1.69E13	0.000	14961.4
CH3+Ccy(CC*CCCC)=CH4+Ccy(CC*CCCCJ)	1.69E13	0.000	14961.4
CH3+Ccy(CC*CCCC)=CH4+Ccy(CJC*CCCC)	4.19E12	0.000	10277.0
CH3+C*cy(CCCCCC)=CH4+C*cy(CCCCJCC)	1.54E13	0.000	14937.5
CH3+C*cy(CCCCCC)=CH4+C*cy(CCCJCCC)	3.07E13	0.000	14937.5
CH3+C*cy(CCCCCC)=CH4+CJcy(C*CCCC)	3.07E13	0.000	14937.5
H+Ccy(CCC*CCC)=H2+CJcy(CCC*CCC)	3.36E14	0.000	12595.3
H+Ccy(CCC*CCC)=H2+Ccy(CCC*CCJC)	1.30E14	0.000	7074.4
H+Ccy(CCC*CCC)=H2+Ccy(CCJCC*CC)	2.33E14	0.000	9942.4
H+Ccy(CCC*CCC)=H2+Ccy(CCJC*CCC)	1.52E14	0.000	7170.0
H+Ccy(CCC*CCC)=H2+Ccy(CJCC*CCC)	1.11E14	0.000	7576.3
H+Ccy(CC*CCCC)=H2+Ccy(CCJC*CCC)	1.30E14	0.000	7074.4
H+Ccy(CC*CCCC)=H2+CJcy(CC*CCCC)	3.36E14	0.000	12595.3
H+Ccy(CC*CCCC)=H2+Ccy(CC*CCCJC)	1.99E14	0.000	9846.8
H+Ccy(CC*CCCC)=H2+Ccy(CC*CCCCJ)	2.33E14	0.000	9942.4
H+Ccy(CC*CCCC)=H2+Ccy(CJC*CCCC)	4.72E13	0.000	5903.3
H+Ccy(C*CCCC)=H2+Ccy(C*CCCJCC)	1.99E14	0.000	9846.8
H+Ccy(C*CCCC)=H2+Ccy(C*CCCCJC)	1.99E14	0.000	9846.8
H+Ccy(C*CCCC)=H2+Ccy(C*CCCCCJ)	1.30E14	0.000	7074.4
H+Ccy(C*CCCC)=H2+Ccy(CJC*CCCC)	1.30E14	0.000	7074.4
H+Ccy(C*CCCC)=H2+CJcy(C*CCCC)	7.28E13	0.000	9177.6
H+C*cy(CCCCCC)=H2+C*cy(CCCCJCC)	1.99E14	0.000	9846.8
H+C*cy(CCCCCC)=H2+C*cy(CCCJCCC)	3.98E14	0.000	9846.8
H+C*cy(CCCCCC)=H2+CJcy(C*CCCC)	2.60E14	0.000	7074.4
OH+Ccy(CCC*CCC)=H2O+Ccy(CCC*CCJC)	5.20E5	2.300	-1362.3

OH+Ccy (CCC*CCC)=H2O+Ccy (CCJC*CCC)	5.20E5	2.300	-1362.3
OH+Ccy (C*CCCC)=H2O+Ccy (C*CCCCJ)	5.20E5	2.300	-1362.3
OH+Ccy (C*CCCC)=H2O+Ccy (CJC*CCCC)	5.20E5	2.300	-1362.3
OH+Ccy (C*CCCC)=H2O+CJcy (C*CCCC)	7.80E5	2.300	-1362.3
OH+Ccy (CC*CCCC)=H2O+Ccy (CCJC*CCC)	5.20E5	2.300	-1362.3
OH+Ccy (CC*CCCC)=H2O+Ccy (CJC*CCCC)	2.60E5	2.300	-1362.3
OH+C*cy (CCCCC)=H2O+CJcy (C*CCCC)	1.04E6	2.300	-1362.3
H2O+Ccy (CCC*CCC)=H2O2+Ccy (CCC*CCJC)	5.12E-2	4.400	13546.5
H2O+Ccy (CCC*CCC)=H2O2+Ccy (CCJC*CCC)	5.12E-2	4.400	13546.5
H2O+Ccy (CC*CCCC)=H2O2+Ccy (CCJC*CCC)	5.12E-2	4.400	13546.5
H2O+Ccy (CC*CCCC)=H2O2+Ccy (CJC*CCCC)	2.56E-2	4.400	13546.5
H2O+Ccy (C*CCCC)=H2O2+Ccy (C*CCCCJ)	5.12E-2	4.400	13546.5
H2O+Ccy (C*CCCC)=H2O2+Ccy (CJC*CCCC)	5.12E-2	4.400	13546.5
H2O+Ccy (C*CCCC)=H2O2+CJcy (C*CCCC)	7.68E-2	4.400	13546.5
H2O+C*cy (CCCCC)=H2O2+CJcy (C*CCCC)	1.02E-1	4.400	13546.5
C*CCCC (C) CJ=Ccy (CCCCJCC)	1.04E10	0.000	10372.6
Ccy (CCC*CCC)+H=Ccy (CCCJCCC)	6.75E13	0.000	4803.9
DUP			
Ccy (CCC*CCC)+H=Ccy (CCCCJCC)	6.75E13	0.000	4803.9
Ccy (CCC*CCC)+H=Ccy (CCCJCCC)	6.75E13	0.000	4803.9
DUP			
Ccy (CC*CCCC)+H=Ccy (CCCJCCC)	6.75E13	0.000	4803.9
DUP			
Ccy (CC*CCCC)+H=Ccy (CCJCCCC)	6.75E13	0.000	4803.9
DUP			
Ccy (C*CCCC)+H=Ccy (CCJCCCC)	1.79E13	0.000	5616.5
DUP			
Ccy (C*CCCC)+H=Ccy (CJCCCC)	7.62E13	0.000	4206.4
Ccy (C*CCCC)+H=Ccy (CCJCCCC)	1.79E13	0.000	5616.5
DUP			
Ccy (CC*CCCC)+H=Ccy (CCJCCCC)	6.75E13	0.000	4803.9
DUP			
Ccy (CC*CCCC)+H=Ccy (CCCJCCC)	6.75E13	0.000	4803.9
DUP			
C*cy (CCCCC)+H=Ccy (CJCCCC)	1.26E14	0.000	3250.4
C*cy (CCCCC)+H=CJcy (CCCCC)	3.42E13	0.000	6190.1
C*CC (C) CCCJ=Ccy (CCJCCCC)	1.04E10	0.000	10372.6
C*CCC (C) CCJ=Ccy (CCCJCCC)	1.04E10	0.000	10372.6
CJCCCC*CC=Ccy (CCJCCCC)	1.04E10	0.000	11878.3
CCJCCCC*C=Ccy (CCCJCCC)	5.22E9	0.000	9249.3
C*CC (C) CC*C+H=CCJCC (C) C*C	5.56E13	0.000	3847.9
DUP			
C*CC (C) CC*C+H=C*CC (C) CCCJ	6.46E13	0.000	5377.5
DUP			
C*CC (C) CC*C+H=C*CCC (C) CJC	5.56E13	0.000	3847.9
DUP			
C*CC (C) CC*C+H=C*CCC (C) CCJ	6.46E13	0.000	5377.5
DUP			
C*CC (C) CC*C+H=CCJCC (C) C*C	5.56E13	0.000	3847.9
DUP			
C*CC (C) CC*C+H=C*CC (C) CCCJ	6.46E13	0.000	5377.5
DUP			
C*CC (C) CC*C+H=C*CCC (C) CJC	5.56E13	0.000	3847.9
DUP			
C*CC (C) CC*C+H=C*CCC (C) CCJ	6.46E13	0.000	5377.5
DUP			
C*CCCC*CC+H=CC*CCCCJC	5.56E13	0.000	3847.9
DUP			

C*CCCC*CC+H=CC*CCCCJC	5.56E13	0.000	3847.9	
DUP				
C*CCCC*CC+H=CJCCCC*CC	6.46E13	0.000	5377.5	
DUP				
C*CCCC*CC+H=CJCCCC*CC	6.46E13	0.000	5377.5	
DUP				
C*CCCC*CC+H=C*CCCCJCC	6.75E13	0.000	4803.9	
C*CCCC*CC+H=CCJCCCC*C	6.75E13	0.000	4803.9	
C*CcyCC*CC*C=C*CcyC*CC*CC		7.04E8	1.200	24808.2
C*CcyC*CC*CC=C*CcyC*CCC*C		5.52E6	2.100	25095.0
C2H3+C*CcyC*CC*CC=>C2H4+C7H7_13	5114.6	1.73E13	0.000	
C2H3+C*CcyC*CCC*C=>C2H4+C7H7_13	5114.6	1.73E13	0.000	
C2H3+C*CcyCC*CC*C=>C2H4+C7H7_13	5114.6	8.66E12	0.000	
C2H5+C*CcyC*CC*CC=>C2H6+C7H7_13	11209.1	2.89E12	0.000	
C2H5+C*CcyC*CCC*C=>C2H6+C7H7_13	11209.1	2.89E12	0.000	
C2H5+C*CcyCC*CC*C=>C2H6+C7H7_13	11209.1	1.45E12	0.000	
C3H3+C*CcyC*CC*CC=>C3H4-A+C7H7_13	18498.6	1.02E13	0.000	
C3H3+C*CcyC*CC*CC=>C3H4-P+C7H7_13	18498.6	1.02E13	0.000	
C3H3+C*CcyC*CCC*C=>C3H4-A+C7H7_13	18498.6	1.02E13	0.000	
C3H3+C*CcyC*CCC*C=>C3H4-P+C7H7_13	18498.6	1.02E13	0.000	
C3H3+C*CcyCC*CC*C=>C3H4-A+C7H7_13	18498.6	5.11E12	0.000	
C3H3+C*CcyCC*CC*C=>C3H4-P+C7H7_13	18498.6	5.11E12	0.000	
C3H5-A+C*CcyC*CC*CC=>C3H6+C7H7_13		3.01E+02	2.970	9160
C3H5-A+C*CcyC*CCC*C=>C3H6+C7H7_13		3.01E+02	2.970	9160
C3H5-A+C*CcyCC*CC*C=>C3H6+C7H7_13		3.01E+02	2.970	9160
C3H5-S+C*CcyC*CC*CC=>C3H6+C7H7_13	5114.6	1.73E13	0.000	
C3H5-S+C*CcyC*CCC*C=>C3H6+C7H7_13	5114.6	1.73E13	0.000	
C3H5-S+C*CcyCC*CC*C=>C3H6+C7H7_13	5114.6	8.66E12	0.000	
C3H5-T+C*CcyC*CC*CC=>C3H6+C7H7_13	6118.4	1.28E13	0.000	
C3H5-T+C*CcyC*CCC*C=>C3H6+C7H7_13	6118.4	1.28E13	0.000	
C3H5-T+C*CcyCC*CC*C=>C3H6+C7H7_13	6118.4	6.42E12	0.000	
CH3+C*CcyC*CC*CC=>CH4+C7H7_13	9918.5	1.78E13	0.000	
CH3+C*CcyC*CCC*C=>CH4+C7H7_13	9918.5	1.78E13	0.000	
CH3+C*CcyCC*CC*C=>CH4+C7H7_13	9918.5	8.92E12	0.000	
H+C*CcyC*CC*CC=>H2+C7H7_13		2.01E14	0.000	6190.1
H+C*CcyC*CCC*C=>H2+C7H7_13		2.01E14	0.000	6190.1
H+C*CcyCC*CC*C=>H2+C7H7_13		5.38E13	0.000	5401.4

OH+C*CcyC*CC*CC=>H2O+C7H7_13	5.20E5	2.300	-1362.3
OH+C*CcyC*CCC*C=>H2O+C7H7_13	5.20E5	2.300	-1362.3
OH+C*CcyCC*CC*C=>H2O+C7H7_13	2.60E5	2.300	-1362.3
H02+C*CcyC*CC*CC=>H2O2+C7H7_13 13546.5	5.12E-2	4.400	
H02+C*CcyC*CCC*C=>H2O2+C7H7_13 13546.5	5.12E-2	4.400	
H02+C*CcyCC*CC*C=>H2O2+C7H7_13 13546.5	2.56E-2	4.400	
C*CcyC*CC*CC+H=CC*cy (CCJC*CC) 2748.5	5.03E13	0.000	
C*CcyC*CC*CC+H=CJCyC*CC*CC	7.85E13	0.000	5951.1
C*CcyC*CCC*C+H=CC*cy (CCJCC*C) 2748.5	5.03E13	0.000	
C*CcyC*CCC*C+H=CJCyC*CCC*C	7.85E13	0.000	5951.1
C*C (CJ)CC*C=C3H5-A+C3H4-A	9.28E+14	0.00	48708.2
C*C (CJ)CC*C=C6H9r_R5_7	1.50E11	0.000	24712.6
CJ*C (C)CC*C=C6H9r_R5	3.74E10	0.000	14507.3
C*CCC*CJC=C6H9r_R5	3.74E10	0.000	14363.9
CJ*C (C)CC*C=C3H5-A+C3H4-P	2.28E14	0.000	24927.7
C*CCC*CJC=C3H5-A+C3H4-P	4.00E14	0.000	26242.2
C2H3+C6H5CC*CC=C2H4+C6H5CCJC*C	7.46E12	0.000	9034.2
C2H3+C6H5CC*CC=C2H4+C6H5CJC*CC	1.70E13	0.000	15367.7
C2H3+C6H5C*CCC=C2H4+C6H5C*CCCJ	3.01E13	0.000	12882.1
C2H3+C6H5C*CCC=C2H4+C6H5CJC*CC	1.61E13	0.000	7361.2
C2H3+C6H5CC*C=C2H4+C6H5CJC*C	1.70E13	0.000	15367.7
C2H3+C6H5CC=C2H4+C6H5CCJ	3.01E13	0.000	12882.1
C2H3+C6H5CC=C2H4+C6H5CJC	5.40E12	0.000	8771.3
C2H3+C6H5CCC*C=C2H4+C6H5CCJC*C	1.61E13	0.000	7361.2
C2H3+C6H5CCC*C=C2H4+C6H5CJCC*C	5.40E12	0.000	8771.3
C2H3+C6H5CCC=C2H4+C6H5CCCJ	2.29E13	0.000	12451.9
C2H3+C6H5CCC=C2H4+C6H5CCJC	2.15E13	0.000	10587.7
C2H3+C6H5CCC=C2H4+C6H5CJCC	4.12E12	0.000	8341.1
C2H3+C7H8=C2H4+C7H7	7.72E12	0.000	11304.7
C2H3+C6H5C*CC=C2H4+C6H5CJC*C	7.46E12	0.000	9034.2
C2H5+C6H5CC*CC=C2H6+C6H5CCJC*C	1.25E12	0.000	15128.7
C2H5+C6H5CC*CC=C2H6+C6H5CJC*CC	2.85E12	0.000	21462.2
C2H5+C6H5C*CCC=C2H6+C6H5C*CCCJ	4.98E12	0.000	18976.6
C2H5+C6H5C*CCC=C2H6+C6H5CJC*CC	2.69E12	0.000	13455.7
C2H5+C6H5CC*C=C2H6+C6H5CJC*C	2.85E12	0.000	21462.2
C2H5+C6H5CC=C2H6+C6H5CCJ	4.94E12	0.000	18976.6
C2H5+C6H5CC=C2H6+C6H5CJC	9.02E11	0.000	14865.8
C2H5+C6H5CCC*C=C2H6+C6H5CCJC*C	2.69E12	0.000	13455.7
C2H5+C6H5CCC*C=C2H6+C6H5CJCC*C	9.02E11	0.000	14865.8
C2H5+C6H5CCC=C2H6+C6H5CCCJ	3.78E12	0.000	18546.4
C2H5+C6H5CCC=C2H6+C6H5CCJC	3.59E12	0.000	16682.2
C2H5+C6H5CCC=C2H6+C6H5CJCC	6.88E11	0.000	14435.6
C2H5+C7H8=C2H6+C7H7	1.29E12	0.000	17399.2
C2H5+C6H5C*CC=C2H6+C6H5CJC*C	1.25E12	0.000	15128.7
C3H5-A+C6H5CC*CC=C3H6+C6H5CCJC*C	1.66E13	0.000	26098.8
C3H5-A+C6H5CC*CC=C3H6+C6H5CJC*CC	3.79E13	0.000	32432.3
C3H5-A+C6H5C*CCC=C3H6+C6H5C*CCCJ	5.53E13	0.000	29946.7
C3H5-A+C6H5C*CCC=C3H6+C6H5CJC*CC	3.58E13	0.000	24425.8
C3H5-A+C6H5CC*C=C3H6+C6H5CJC*C	3.79E13	0.000	32432.3
C3H5-A+C6H5CC=C3H6+C6H5CCJ	5.47E13	0.000	29946.7
C3H5-A+C6H5CC=C3H6+C6H5CJC	1.20E13	0.000	25835.9
C3H5-A+C6H5CCC*C=C3H6+C6H5CCJC*C	3.58E13	0.000	24425.8
C3H5-A+C6H5CCC*C=C3H6+C6H5CJCC*C	1.19E13	0.000	25835.9

C3H5-A+C6H5CCC=C3H6+C6H5CCCJ4.19E13	0.000	29516.5
C3H5-A+C6H5CCC=C3H6+C6H5CCJC4.17E13	0.000	27652.3
C3H5-A+C6H5CCC=C3H6+C6H5CJCC9.08E12	0.000	25405.7
C3H5-A+C7H8=C3H6+C7H7 1.65E13	0.000	28369.3
C3H5-A+C6H5C*CC=C3H6+C6H5CJC*C 1.44E13	0.000	26098.8
CH3+C6H5CC*CC=CH4+C6H5CCJC*C7.68E12	0.000	13838.1
CH3+C6H5CC*CC=CH4+C6H5CJC*CC1.76E13	0.000	20171.6
CH3+C6H5C*CCC=CH4+C6H5C*CCCJ3.10E13	0.000	17686.0
CH3+C6H5C*CCC=CH4+C6H5CJC*CC1.66E13	0.000	12165.1
CH3+C6H5CC*C=CH4+C6H5CJC*C 1.76E13	0.000	20171.6
CH3+C6H5CC=CH4+C6H5CCJ 3.10E13	0.000	17686.0
CH3+C6H5CC=CH4+C6H5CJC 5.56E12	0.000	13575.2
CH3+C6H5CCC*C=CH4+C6H5CCJC*C1.66E13	0.000	12165.1
CH3+C6H5CCC*C=CH4+C6H5CJCC*C5.56E12	0.000	13575.2
CH3+C6H5CCC=CH4+C6H5CCCJ 2.36E13	0.000	17255.8
CH3+C6H5CCC=CH4+C6H5CCJC 2.22E13	0.000	15391.6
CH3+C6H5CCC=CH4+C6H5CJCC 4.24E12	0.000	13145.0
CH3+C7H8=CH4+C7H7 7.95E12	0.000	16108.6
CH3+C6H5C*CC=CH4+C6H5CJC*C 7.68E12	0.000	13838.1
H+C6H5CC*CC=H2+C6H5CCJC*C 7.28E13	0.000	9177.6
H+C6H5CC*CC=H2+C6H5CJC*CC 6.38E14	0.000	15869.6
H+C6H5C*CCC=H2+C6H5C*CCCJ 2.87E14	0.000	12499.7
H+C6H5C*CCC=H2+C6H5CJC*CC 1.59E14	0.000	7361.2
H+C6H5CC*C=H2+C6H5CJC*C 6.38E14	0.000	15869.6
H+C6H5CC=H2+C6H5CCJ 3.51E14	0.000	12786.5
H+C6H5CC=H2+C6H5CJC 1.00E14	0.000	9583.9
H+C6H5CCC*C=H2+C6H5CCJC*C 1.59E14	0.000	7361.2
H+C6H5CCC*C=H2+C6H5CJCC*C 8.20E13	0.000	9297.1
H+C6H5CCC=H2+C6H5CCCJ 2.87E14	0.000	12499.7
H+C6H5CCC=H2+C6H5CCJC 2.44E14	0.000	10133.6
H+C6H5CCC=H2+C6H5CJCC 8.20E13	0.000	9297.1
H+C7H8=H2+C7H7 8.79E13	0.000	11328.6
H+C6H5C*CC=H2+C6H5CJC*C 7.28E13	0.000	9177.6
C6H5C*CC*C+H=C6H5C*CCCJ 7.85E13	0.000	5951.1
DUP		
C6H5C*CC*C+H=C6H5C*CCCJ 7.85E13	0.000	5951.1
DUP		
C6H5C*CC*C+H=C6H5CCJC*C 2.19E13	0.000	6453.0
C6H5C*CC*C+H=C6H5CJC*CC 5.03E13	0.000	2748.5
C6H5C*CC*C+H=C6H5CJCC*C 2.00E13	0.000	6453.0
C6H5CC*CC+H=C6H5CCCJ 6.75E13	0.000	4803.9
C6H5CC*CC+H=C6H5CCJCC 6.75E13	0.000	4803.9
C6H5C*CCC+H=C6H5CCJCC 2.42E13	0.000	7552.4
C6H5C*CCC+H=C6H5CJCCC 1.64E13	0.000	5879.4
C6H5C2H3+H=C6H5CCJ 2.31E13	0.000	8126.0
C6H5C2H3+H=C6H5CJC 1.35E13	0.000	4923.4
C6H5CC*C+H=C6H5CCCJ 6.46E13	0.000	5377.5
C6H5CC*C+H=C6H5CCJC 5.56E13	0.000	3847.9
C6H5CCC*C+H=C6H5CCCCJ 6.46E13	0.000	5377.5
C6H5CCC*C+H=C6H5CCCJC 5.56E13	0.000	3847.9
C6H5C*CC+H=C6H5CCJC 2.42E13	0.000	7552.4
C6H5C*CC+H=C6H5CJCC 1.64E13	0.000	5879.4
C6H5CCCCJ=C2H4+C6H5CCJ 5.05E13	0.000	28632.2
C6H5CCCJ=C2H4+C7H7 9.92E12	0.000	22131.4
C6H5CCCJC=C3H6+C7H7 6.02E12	0.000	21940.2
C6H5CCJCC=CH3+C6H5CC*C 4.27E13	0.000	30520.3
C6H5CJCC*C=C2H3+C6H5C2H3 1.65E14	0.000	44525.7
C6H5CJCC=CH3+C6H5C2H3 1.68E14	0.000	38694.1

C6H5CJCCC=C2H5+C6H5C2H3	1.21E14	0.000	36614.8	
C7H7+C6H10=C7H8+C6H9-A	3.38E13	0.000	22346.5	
C*CCJ*CCC*C=C3H5-A+C4H4		1.32E14	0.000	33053.7
C*CCJ*CCC*C=C*Ccy(C*CCCJC)		3.74E10	0.000	18164.0
C*CcyC*CC*CC+H=C*Ccy(C*CCCJC)		8.20E13	0.000	
5377.5				
C*CcyC*CCC*C+H=C*Ccy(C*CCCJC)		8.20E13	0.000	
5377.5				
C*CC*CCC*C+H=C*CCC*CCJC	5.03E13	0.000	2748.5	
C*CC*CCC*C+H=C*CCCCJC*C	6.11E13	0.000	3704.5	
C*CC*CCC*C+H=C7H11r_olef_29	6.46E13	0.000	5377.5	
DUP				
C*CC*CCC*C+H=C7H11r_olef_29	6.46E13	0.000	5377.5	
DUP				
C*CC*CCC*C+H=C*CCCJCC*C	8.20E13	0.000	5377.5	
C*CC*CCC*C+H=C*CC*CCCJC	5.56E13	0.000	3847.9	
DUP				
C*CC*CCC*C+H=C*CC*CCCJC	5.56E13	0.000	3847.9	
DUP				
C*CC*CCC*C+H=C7H11r_olef_27	7.85E13	0.000	5951.1	
DUP				
C*CC*CCC*C+H=C7H11r_olef_27	7.85E13	0.000	5951.1	
DUP				
C*CC*CC*CC+H=C*CCC*CCJC	7.43E13	0.000	4278.1	
C*CC*CC*CC+H=CC*CC*CCCJ	7.85E13	0.000	5951.1	
DUP				
C*CC*CC*CC+H=CC*CC*CCCJ	7.85E13	0.000	5951.1	
DUP				
C*CC*CC*CC+H=CC*CC*CCCJ	7.85E13	0.000	5951.1	
DUP				
C*CC*CC*CC+H=C*CC*CCCJC	8.20E13	0.000	5377.5	
DUP				
C*CC*CC*CC+H=C*CC*CCCJC	8.20E13	0.000	5377.5	
DUP				
C*CC*CC*CC+H=C*CCJCC*CC	7.43E13	0.000	4278.1	
DUP				
C*CC*CC*CC+H=C*CCJCC*CC	7.43E13	0.000	4278.1	
DUP				
C*CC*CC*CC+H=CC*CC*CCJC	5.03E13	0.000	2748.5	
C*CC*CC*CC+H=CCC*CC*CCJ	6.11E13	0.000	3704.5	
C7H7+C*CCC*C=>C7H8+C*CC*CCJ		1.82E13	0.000	
20099.9				
C7H7+C*CCCC=>C7H8+C*CCCCJ		2.08E13	0.000	
27437.2				
C7H7+C*CCCC=>C7H8+C*CCCJC		2.09E13	0.000	
25573.0				
C7H7+C*CCCC=>C7H8+C*CCJCC		1.29E13	0.000	
21916.3				
C7H7+C*Ccy(C*CCC*C)=>C7H8+C*CC*cyCCJCC*C		1.82E13	0.000	
20099.9				
C7H7+C*Ccy(C*CCC*C)=>C7H8+C*CCcyCJC*CC*C		1.82E13	0.000	
20099.9				
C7H7+C*CcyC*CC*CC=>C7H8+C7H7_13		1.82E13	0.000	
20099.9				
C7H7+C*cy(CCC*CC)=>C7H8+C*cy(CCJC*CC)		3.63E13	0.000	
20099.9				

C7H7+Ccy (C*CC*CC) =>C7H8+C*cy (CCJC*CC) 24019.5		7.83E12	0.000
C7H7+Ccy (C*CC*CC) =>C7H8+Ccy (CJC*CC*C) 20099.9		1.82E13	0.000
C7H7+Ccy (C*CCC*C) =>C7H8+C*cy (CCJCC*C) 24019.5		7.83E12	0.000
C7H7+Ccy (C*CCC*C) =>C7H8+Ccy (CJC*CC*C) 20099.9		1.82E13	0.000
C7H7+Ccy (CC*CC*C) =>C7H8+CJcy (CC*CC*C) 27867.4		2.74E13	0.000
C7H7+Ccy (CC*CC*C) =>C7H8+Ccy (CJC*CC*C) 18833.2		4.10E12	0.000
C7H7+C4H8-1=>C7H8+C4H71-3 22346.5		1.69E13	0.000
C7H7+C4H8-1=>C7H8+C4H71-4 27867.4		2.74E13	0.000
C7H7+C4H8-2=>C7H8+C4H71-3 24019.5		1.57E13	0.000
C7H7+C*CC*CC=>C7H8+C*CC*CCJ 24019.5		7.83E12	0.000
C7H7+cy (C*CC*CCC) =>C7H8+cy (C*CC*CCJC) 22346.5		3.38E13	0.000
C7H7+cy (C*CCC*CC) =>C7H8+cy (C*CC*CCJC) 20099.9		3.63E13	0.000
C7H7+cy (C*CCCC) =>C7H8+C5H7 21916.3		2.57E13	0.000
C7H7+cy (C*CCCC) =>C7H8+cy (C*CCCCJC) 25573.0		2.04E13	0.000
O2+C5H7=JOOcy (CC*CCC)	2.90E7	1.590	1080.3
JOOcy (CC*CCC) =C5H6+HO2	5.77E9	0.930	29799.3
C5H7+HO2=HOOcy (CC*CCC)	1.68E10	0.600	-2105.6
HOOcy (CC*CCC) =Jocy (CC*CCC) +OH 42857.5		1.59E20	-1.500
Jocy (CC*CCC) =O*cy (CC*CCC) +H	5.87E9	1.000	18548.8
cy (C*CC*CCJC) +HO2=HOOcy (CC*CCC*C) 2105.6		1.68E10	0.600
cy (C*CC*CCJC) +HO2=HOOcy (CC*CC*CC) 2105.6		1.68E10	0.600
HOOcy (CC*CCC*C) =Jocy (CC*CCC*C) +OH 42857.5		1.59E20	-1.500
HOOcy (CC*CC*CC) =Jocy (CC*CC*CC) +OH 42857.5		1.59E20	-1.500
Jocy (CC*CC*CC) =O*cy (CC*CC*CC) +H 18548.8		5.87E9	1.000
Jocy (CC*CCC*C) =O*cy (CC*CCC*C) +H 18548.8		5.87E9	1.000
C5H6+OH=HOcyCCJCC*C	1.56E8	1.290	-2652.9
C5H6+OH=HOcyCCJC*CC	1.56E8	1.290	-2652.9
cy (C*CC*CCC) +OH=HOcyCCJCCC*C	1.56E8	1.290	-2652.9
cy (C*CC*CCC) +OH=HOcy (CCJC*CCC)	1.56E8	1.290	-2652.9
cy (C*CCC*CC) +OH=HOcy (CCJCC*CC)	3.12E8	1.290	-2652.9
cy (C*CCCC) +OH=HOcyCCJCCC	1.56E8	1.290	-2652.9
DUP			
cy (C*CCCC) +OH=HOcyCCJCCC	1.56E8	1.290	-2652.9
DUP			
cy (C*CCCC) +OH=HOcy (CCJCCCC)	1.56E8	1.290	-2652.9
DUP			
cy (C*CCCC) +OH=HOcy (CCJCCCC)	1.56E8	1.290	-2652.9

DUP
O2+HOcyCCJCC*C=JOOcyCCOHC*CC 7.54E14 -0.920 -129.1
O2+HOcyCCJCCC=JOOcyCCOHCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcyCCJCCC=JOOcyCCOHCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcyCCJCCC=JOOcyCCOHCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcyCCJCCC=JOOcyCCOHCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcy(CCJCCCC)=JOOcyCCOHCCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcy(CCJCCCC)=JOOcyCCOHCCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcy(CCJCCCC)=JOOcyCCOHCCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcy(CCJCCCC)=JOOcyCCOHCCCC 7.54E14 -0.920 -129.1
DUP
O2+HOcyCCJCCC*C=JOOcyCCOHC*CCC 7.54E14 -0.920 -129.1
O2+HOcy(CCJCC*CC)=JOOcyCCOHCC*CC 7.54E14 -0.920 -129.1
O2+HOcyCCJC*CC=JOOcyCCOHCC*C 1.45E7 1.590 1080.3
O2+HOcyCCJC*CC=JOOcyCC*CCOHC 1.45E7 1.590 1080.3
O2+HOcy(CCJC*CCC)=JOOcyCCOHCCC*C 1.45E7 1.590 1080.3
O2+HOcy(CCJC*CCC)=JOOcyCC*CCOHC 1.45E7 1.590 1080.3
JOOcyCCOHCC*C=JOcy(CCPC*CC) 2.91E12 -0.230 22298.7
JOOcyCCOHC*CC=JOcyCCPCC*C 2.91E12 -0.230 22298.7
JOOcyCCOHCCC=JOcy(CCPCCC) 2.91E12 -0.230 22298.7
JOOcyCCOHCCCC=JOcyCCPCCCC 2.91E12 -0.230 22298.7
JOOcyCCOHCC*CC=JOcy(CCPCC*CC) 2.91E12 -0.230 22298.7
JOOcyCCOHCCC*C=JOcyCCPC*CCC 2.91E12 -0.230 22298.7
JOOcyCCOHC*CCC=JOcyCCPCCC*C 2.91E12 -0.230 22298.7
JOcy(CCPC*CC)=O*CCPCJC*C 3.00E13 0.220 14098.6
JOcy(CCPC*CC)=O*CCC*CCJOOH 3.00E13 0.220 14098.6
JOcyCCPCC*C=O*CC*CCCJOOH 3.00E13 0.220 14098.6
JOcy(CCPCCC)=O*CCCCCJOOH 3.00E13 0.220 14098.6
JOcy(CCPCCC)=O*CCPCCCJ 3.00E13 0.220 14098.6
JOcyCCPCCCC=O*CCCCCJOOH 3.00E13 0.220 14098.6
JOcyCCPCCCC=O*CCPCCCCJ 3.00E13 0.220 14098.6
JOcy(CCPCC*CC)=O*CCPCCJC*C 3.00E13 0.220 14098.6
JOcy(CCPCC*CC)=O*CCC*CCCJOOH 3.00E13 0.220 14098.6
JOcyCCPC*CCC=O*CCPC*CCCJ 3.00E13 0.220 14098.6
JOcyCCPC*CCC=O*CCCC*CCJOOH 3.00E13 0.220 14098.6
JOcyCCPCCC*C=O*CC*CCCCJOOH 3.00E13 0.220 14098.6
O*CCC*CCJOOH=>C5H6O2_1+OH 9.00E14 0.000 1500.9
O*CC*CCCJOOH=>C5H6O2_1+OH 9.00E14 0.000 1500.9
O*CCCCCJOOH=>O*CCCCC*O+OH 9.00E14 0.000 1500.9
O*CCCCCJOOH=>O*CCCCC*O+OH 9.00E14 0.000 1500.9
O*CCC*CCCJOOH=>O*CCC*CCC*O+OH 9.00E14 0.000 1500.9
O*CCCC*CCJOOH=>O*CC*CCCC*O+OH 9.00E14 0.000 1500.9
O*CC*CCCCJOOH=>O*CC*CCCC*O+OH 9.00E14 0.000 1500.9
O*CCPCJC*C=>C5H6O_1+HO 2.183E10 0.790 15099.6
C*CCCC*O+H=CCJCCC*O 5.56E13 0.000 3847.9
C*CCCC*O+H=CJCCCC*O 6.46E13 0.000 5377.5
CCJCCC*O=C3H6+CH2CHO 2.07E13 0.000 22824.5
CJCCCC*O=C2H4+CH2CH2CHO 5.05E13 0.000 28632.2
C*CCJCCy(COC)=C4H6+C2H3O1-2 1.78E14 0.000 32671.3
C3H5-A+C*CCCy(COC)=C3H6+C*CCJCCy(COC) 2.73E13 0.000 23995.6
C3H5-A+C*CC*CCC*O=C3H6+C*CC*CCJC*O 3.79E13 0.000 32432.3

CH3+C*CCCey (COC) =CH4+C*CCJCCey (COC)	1.26E13	0.000	11734.9
CH3+C*CC*CCC*O=CH4+C*CC*CCJC*O	1.76E13	0.000	20171.6
H+C*CCCey (COC) =H2+C*CCJCCey (COC)	1.59E14	0.000	7361.2
H+C*CC*CCC*O=H2+C*CC*CCJC*O	2.01E14	0.000	6190.1
OH+C*CCCey (COC) =H2O+C*CCJCCey (COC)	5.20E5	2.300	-1362.3
OH+C*CC*CCC*O=H2O+C*CC*CCJC*O	5.20E5	2.300	-1362.3
HO2+C*CCCey (COC) =H2O2+C*CCJCCey (COC)	5.12E-2	4.400	13546.5
HO2+C*CC*CCC*O=H2O2+C*CC*CCJC*O	5.12E-2	4.400	13546.5
C*CC*CCJC*O=>C*CC*CCJ+CO	6.100E+005	0.920	-1120.0
C*CCCC*O+OH=HOCCJCCC*O	7.80E7	1.290	-2652.9
C*CCCC*O+OH=CJC (OH) CCC*O	7.80E7	1.290	-2652.9
DUP			
C*CCCC*O+OH=CJC (OH) CCC*O	7.80E7	1.290	-2652.9
DUP			
CJC (OH) CCC*O=C2H3OH+CH2CH2CHO	4.41E13	0.000	27461.1
HOCCJCCC*O=C3H5OH+CH2CHO	2.07E13	0.000	22824.5
C*CCCey (COC) +OH=HOCCJCCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +OH=CJC (OH) CCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +OH=CJC (OH) CCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +OH=HOCCJCCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +OH=CJC (OH) CCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +OH=CJC (OH) CCey (COC)	7.80E7	1.290	-2652.9
DUP			
C*CCCey (COC) +H=CCJCCey (COC)	5.56E13	0.000	3847.9
DUP			
C*CCCey (COC) +H=CJCCey (COC)	6.46E13	0.000	5377.5
DUP			
C*CCCey (COC) +H=CCJCCey (COC)	5.56E13	0.000	3847.9
DUP			
C*CCCey (COC) +H=CJCCey (COC)	6.46E13	0.000	5377.5
DUP			
C*CC*CCC*O+OH=HOCCJC*CCC*O	7.80E7	1.290	-2652.9
C*CC*CCC*O+OH=CJC (OH) C*CCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=CJC (OH) C*CCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=CJC (OH) C*CCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=CJC (OH) C*CCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=C*CC (OH) CJCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=C*CC (OH) CJCC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=C*CCJC (OH) CC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+OH=C*CCJC (OH) CC*O	7.80E7	1.290	-2652.9
DUP			
C*CC*CCC*O+H=CC*CCJCC*O	5.03E13	0.000	2748.5
C*CC*CCC*O+H=CJCC*CCC*O	7.85E13	0.000	5951.1
DUP			
C*CC*CCC*O+H=CJCC*CCC*O	7.85E13	0.000	5951.1
DUP			

C*CC*CCC*O+H=C*CCCJCC*O	8.20E13	0.000	5377.5	
C*CC*CCC*O+H=C*CCJCCC*O	6.11E13	0.000	3704.5	
HOCCJCCcy (COC)=C3H5OH+C3H5O	3.07E13	0.000	28441.0	
CJC (OH) CCcy (COC)=>C2H3OH+C2H4+C2H3O1-2	4.41E13	0.000	27461.1	
CCJCCcy (COC)=C3H6+C3H5O	3.07E13	0.000	28441.0	
CJCCCcy (COC)=>C2H4+C2H4+C2H3O1-2	5.05E13	0.000	28632.2	
HOCCJC*CCC*O=C*CC*CCOH+HCO	2.89E14	0.000	33268.8	
CJC (OH) C*CCC*O=C2H3OH+C4H5Or_olef	6.93E13	0.000	36543.1	
C*CC (OH) CJCC*O=C2H3+OC4H6O	4.20E13	0.000	36351.9	
C*CC (OH) CJCC*O=C*CC (OH) C*C+HCO	5.17E13	0.000	24330.2	
C*CCJC (OH) CC*O=C4H6O_olef_1+CH2CHO	1.01E14	0.000	30592.0	
CC*CCJCC*O=C*CC*CC+HCO	2.89E14	0.000	33268.8	
CJCC*CCC*O=C2H4+C4H5Or_olef	6.93E13	0.000	36543.1	
C*CCCJCC*O=C*CCC*C+HCO	5.17E13	0.000	24330.2	
C*CCCJCC*O=C2H3+C*CCC*O	4.20E13	0.000	36351.9	
C*CCJCCC*O=C4H6+CH2CHO	1.16E14	0.000	31763.1	
!O2+C4H71-4=C*CCCCOJ	5.20E11	0.230	-1579.8	
!C*CCCCOJ=C4H6+HO2	3.16E10	0.637	27578.2	
O2+cy (CJCCCC)=JOOcy (CCCC)	1.51E15	-0.920	-129.1	
JOOcy (CCCC)=cy (C*CCCC)+HO2	1.15E10	0.930	29799.3	
cy (CJCCCC)+O2=cy (C*CCCC)+HO2	7.90E+12	0.000	5000.	
!CPcy (CCJC*CC)=cy (CC*CcyCOCC)+OH	4.58E+15	-1.080	18440	
!cy (CC*CcyCOCC)=C5H6+CH2O	6.00E+14	0.000	60000.0	
C*CC*CC*CJ=cy (C*CC*CCJC)	5.22E9	0.000	4493.2	
!C*CC*CC*CJ=C2H2+C4H5-N	3.52E13	0.000	30711.5	
O2+CJcy (CC*CCC)=JOOcCy (CC*CCC)	5.20E11	0.230	-	
1579.8				
JOOcCy (CC*CCC)=C*cy (CC*CCC)+HO2	1.58E10	0.637		
27578.2				
cy (C*CCJCCC)+HO2=HOOcy (CC*CCCC)	1.68E10	0.600	-2105.6	
DUP				
cy (C*CCJCCC)+HO2=HOOcy (CC*CCCC)	1.68E10	0.600	-2105.6	
DUP				
cy (C*CCCJCC)+HO2=HOOcy (CCC*CCC)	8.39E9	0.600	-2105.6	
HOOcy (CC*CCCC)=JOOcy (CC*CCCC)+OH	1.59E20	-1.500	42857.5	
HOOcy (CCC*CCC)=JOOcy (CCC*CCC)+OH	1.59E20	-1.500	42857.5	
CJCCC*CC*O=C2H4+C*CCJC*O	1.51E13	0.000	20745.2	
JOOcy (CC*CCCC)=CJCCC*CC*O	3.00E13	0.220	14098.6	
JOOcy (CCC*CCC)=C*CCJCCC*O	3.00E13	0.220	14098.6	
JOOcy (CCC*CCC)=CJCC*CCC*O	3.00E13	0.220	14098.6	
CJCC*CC*COH=HOOcy (CCJC*CCC)	1.04E10	0.000	10516.0	
C*CCJCC*COH=HOOcy (CCJCC*CC)	5.22E9	0.000	20291.1	
CJCC*CC*COH=HOCJcyCC*CCC	2.80E10	0.000	10641.2	
C*CCJCC*COH=HOCJcyCCC*CC	2.80E10	0.000	17715.6	
HOCOOJcyCC*CCC=HOC*cyCC*CCC+HO2	1.58E10	0.637	27578.2	
O2+HOCJcyCCC*CC=HOCOOJcyCCC*CC	2.02E13	-0.310	-337.0	
O2+HOCJcyCC*CCC=HOCOOJcyCC*CCC	2.02E13	-0.310	-337.0	
HOCOOJcyCCC*CC=O*CcyCCC*CC+HO2	2.60E8	1.128	10630.7	
HOCOOJcyCC*CCC=O*CcyCC*CCC+HO2	2.60E8	1.128	10630.7	
O2+C*CCC*C=HO2+C*CC*CCJ	2.00E13	0.000	25827.1	
O2+C*CC*CC=HO2+C*CC*CCJ	3.00E13	0.000	31428.1	
O2+cy (C*CCCC)=HO2+C5H7	4.00E13	0.000	35997.1	
O2+cy (C*CCCC)=HO2+cy (C*CCCJC)	2.00E13	0.000	49870.7	
C*CCC (C) CJ=Ccy (CCCJCC)	7.48E10	0.000	17662.1	
C*CCC (C) CJ=C*CCC*C+CH3	7.68E13	0.000	30615.9	
C*CCC (C) CJ=C3H5-A+C3H6	1.65E13	0.000	20649.6	
Ccy (C*CCCC)+H=Ccy (CCJCCC)	1.79E13	0.000	5616.5	
DUP				

Ccy (C*CCCC) +H=Ccy (CJCCCC)	7.62E13	0.000	4206.4
Ccy (C*CCCC) +H=Ccy (CCJCCC)	1.79E13	0.000	5616.5
DUP			
C6H10_R5+H=Ccy (CCCJCC)	6.75E13	0.000	4803.9
C6H10_R5+H=Ccy (CCJCCC)	6.75E13	0.000	4803.9
Ccy (CCC*CC) +H=Ccy (CCCJCC)	6.75E13	0.000	4803.9
DUP			
Ccy (CCC*CC) +H=Ccy (CCCJCC)	6.75E13	0.000	4803.9
DUP			
O2+cy (C*CCCJC) =JOOcy (CCC*CC)	3.02E15	-0.920	-129.1
JOOcy (CCC*CC) =C5H6+HO2	6.32E10	0.637	27578.2
CJ*CCC*C=C*CC*CCJ	2.40E12	0.000	29205.8
CH3+C4H8-1=CH4+C4H71-1	1.10E+13	0.000	20172
CH3+C4H8-1=CH4+C4H71-2	1.28E+13	0.000	17973
CH3+C4H8-1=CH4+C4H71-3	1.66E+13	0.000	12165
CH3+C4H8-1=CH4+C4H71-4	3.10E+13	0.000	17686
H+C4H8-1=H2+C4H71-1	1.81E+14	0.000	17232
H+C4H8-1=H2+C4H71-2	1.79E+14	0.000	14340
H+C4H8-1=H2+C4H71-3	1.59E+14	0.000	7361
H+C4H8-1=H2+C4H71-4	3.51E+14	0.000	12787
C3H4-A+H=C3H3+H2	3.70E+07	2.05	6500
CH3+C3H4-A=C3H3+CH4	1.80E+03	2.98	7900
C2H3+C3H4-A=C2H4+C3H3	1.10E+03	3.06	3500
C3H4-P+H=C3H3+H2	2.50E+07	2.03	6200
CH3+C3H4-P=C3H3+CH4	2.58E+03	3.00	8000
C2H3+C3H4-P=C2H4+C3H3	4.70E+02	3.09	3600
CH3+C*CCCC=CH4+C*CJCCC	1.27E13	0.000	17972.8
CH3+C*CCCC=CH4+CJ*CCCC	1.09E13	0.000	20171.6
H+C*CCCC=H2+C*CJCCC	1.79E14	0.000	14340.0
H+C*CCCC=H2+CJ*CCCC	1.81E14	0.000	17231.9
OH+C*CCCC=H2O+CJ*CCCC	9.010E-001	3.941	1637.9
OH+C*CCCC=H2O+C*CJCCC	1.430E+001	3.534	478.1
C*CJCCC=C3H4-A+C2H5	9.18E14	0.000	33507.8
CJ*CCCC=C2H2+NC3H7	5.18E14	0.000	34105.3
C6H11Or_olef_1=HOcy (CCCCJCC)	1.04E10	0.000	10444.3
O2+HOcy (CCCCJCC) =HOcyCCCC (OOJ) CC	3.77E14	-0.920	-129.1
DUP			
O2+HOcy (CCCCJCC) =HOcyCCCC (OOJ) CC	3.77E14	-0.920	-129.1
DUP			
HOcyCCCC (OOJ) CC=HOcy (CCC*CCC) +HO2	1.15E10	0.930	29799.3
HOcy (CCC*CCC) +H=HOcy (CCCCJCC)	6.75E13	0.000	4803.9
C4H71-3+HO2=C*CC (C) OOH	8.39E9	0.600	-2105.6
DUP			
C4H71-3+HO2=C*CC (C) OOH	8.39E9	0.600	-2105.6
DUP			
C4H71-3+HO2=CC*CCOOH	8.39E9	0.600	-2105.6
DUP			
C4H71-3+HO2=CC*CCOOH	8.39E9	0.600	-2105.6
DUP			
C*CC (C) OOH=C4H70+OH	1.59E20	-1.500	42857.5
CC*CCOOH=CC*CCOJ+OH	1.59E20	-1.500	42857.5
C4H70=C2H3CHO+CH3	9.00E13	0.220	14098.6
CC*CCOJ=CH3CHCHCHO+H	3.52E10	1.000	18548.8
C4H70=C2H3COCH3+H	1.76E10	1.000	18548.8
CC*CCOJ=C3H5-S+CH2O	8.10E14	0.000	23890.4
C4H70=C2H3+CH3CHO	8.10E14	0.000	23890.4
C4H6+H=C4H5-N+H2	1.90E+08	1.87	13700
DUP			

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C4H6+H=H2+C4H5-N 5.80E+07 1.98 13100
DUP
C4H6+H=C4H5-I+H2 7.60E+09 1.41 11400
CH3+C4H6=CH4+C4H5-N 3.30E+03 2.88 13900
DUP
CH3+C4H6=CH4+C4H5-N 7.00E+02 2.96 13300
DUP
CH3+C4H6=CH4+C4H5-I 4.30E+04 2.58 11800
C2H3+C4H6=C2H4+C4H5-N 1.10E+02 3.16 7800
DUP
C2H3+C4H6=C2H4+C4H5-N 7.90E+02 3.04 8400
DUP
C2H3+C4H6=C2H4+C4H5-I 7.00E+03 2.79 6700
C2H5+C4H6=C2H6+C4H5-N 1.20E+03 3.01 15500
DUP
C2H5+C4H6=C2H6+C4H5-N 2.20E+02 3.11 15100
DUP
C2H5+C4H6=C2H6+C4H5-I 1.80E+04 2.66 13200
C3H5-A+C4H6=C3H6+C4H5-N 2.30E+03 3.05 26900
DUP
C3H5-A+C4H6=C3H6+C4H5-N 4.30E+04 2.87 27400
DUP
C3H5-A+C4H6=C3H6+C4H5-I 8.20E+05 2.39 24100
CJcy(CCC*CCC)=Ccy(CCJC*CCC) 5.84E+12 0.00 30500
H+C*CC*CC=H2+C*CC*CCJ 7.28E+13 0 1177.6
!CH3+C*CC*CC=CH4+C*CC*CCJ 8.99E+02 2.84 5770
C3H5-A+C*CC*CC=C3H6+C*CC*CCJ 3.51E+00 3.62 12900

C3H5-A+C6H10=C3H6+C6H9-A 7.24E+00 3.600 13300

C4H4+CH3=>C5H6+H 3.91E+12 0.000 8651.8

!O2+C6H10=HO2+C6H9-A 1.19E+20 -1.67 46192.1
O2+C6H10=HO2+C6H9-A 4.00E+13 0.000 33916.9 ! RDB -2 kcal
C*CCJCC+O2<=>C*CC*CC+HO2 1.000E+009 0.000
0.0
CC*CCJC+O2<=>C*CC*CC+HO2 1.000E+009 0.000
0.0

C6H10<=>C3H5-A+C3H5-A 7.244E+047 -9.700
72680.0
PLOG/ 1.0000 7.244E+047 -9.700 72680.0/
PLOG/ 4.0000 6.026E+039 -7.300 69390.0/
PLOG/ 10.0000 3.162E+035 -6.000 67620.0/
! Exp values 1-butene
!C6H10+H=C6H11 2.10E+09 1.400 726.876
!C6H10+H=C*CCCCCJ 1.80E+09 1.400 2307.732
! Genesys
C6H10+H=C6H11 1.11E14 0.000 3847.9
C6H10+H=C*CCCCCJ 1.29E14 0.000 5377.5

!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/
C6H9-A+O2<=>C5H7Or_olef+CH2O 1.190E+015 -
1.010 20128.0 !C3H5-A+O2<=>CH3CO+CH2O

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PLOG/	1.0000	1.190E+015	-1.010	20128.0/	
PLOG/	10.0000	7.140E+015	-1.210	21046.0/	
C6H9-A+O2<=>C*CC (*O) CC*C+OH					1.820E+013 -
0.410	22859.0	!C3H5-A+O2<=>C2H3CHO+OH			
PLOG/	1.0000	1.820E+013	-0.410	22859.0/	
PLOG/	10.0000	2.470E+013	-0.450	23017.0/	

C4H8-1+C3H5-A=C4H71-3+C3H6 13.9 3.45 13500

!C6H10+OH=C*CCCCJCOH	2.34E8	1.290	-2652.9	! x1.5
!DUP				
!C6H10+OH=C*CCCCJCOH	3.56E5	2.180	1063	! x1.5
!DUP				
!C6H10+OH=C6H11Or_Olef_1	0.78E8	1.290	-2652.9	! x0.5
!DUP				
!C6H10+OH=C6H11Or_Olef_1	1.19E5	2.180	1063	! x0.5
!DUP				

C6H10+OH=C*CCCCJCOH	1.56E8	1.290	-2652.9	! x1
DUP				
C6H10+OH=C*CCCCJCOH	2.38E5	2.180	1063	! x1
DUP				
C6H10+OH=C6H11Or_Olef_1	1.56E8	1.290	-2652.9	! x1
DUP				
C6H10+OH=C6H11Or_Olef_1	2.38E5	2.180	1063	! x1
DUP				

!OH+C6H10=H2O+CJ*CCCC*C	1.52E+04	2.80	2193	
!DUP				
!OH+C6H10=H2O+CJ*CCCC*C	2.02E+00	3.51	-101	
!DUP				
!OH+C6H10=H2O+C*CJCCC*C	9.35E+04	2.47	1748	
!DUP				
!OH+C6H10=H2O+C*CJCCC*C	1.14E-06	2.61	-3086	
!DUP				
OH+C6H10=H2O+CJ*CCCC*C	1.80E+00	3.941	1637.9	
OH+C6H10=H2O+C*CJCCC*C	2.86E+01	3.534	478.1	

C6H10+O<=>C*CCCCJ+HCO	2.71E+07	1.880	183	
C6H10+O<=>C6H9-A+OH	6.99E+11	0.700	5884	
C6H10+O<=>CJ*CCCC*C+OH	2.40E+11	0.700	8959	
C6H10+O<=>C*CJCCC*C+OH	1.21E+11	0.700	7632	

CJ*CCCC*C+O2=>C*CCCC*O+HCO	3.10E+31	-5.944	5748.4	
!! C3H5-S+O2<=>CH3CHO+HCO				
CJ*CCCC*C+O2=>C3H5-A+C2H3CHO+O	5.38E+18	-2.140	5142.9	
!! C3H5-S+O2<=>CH3CHCHO+O				
CJ*CCCC*C+O2=>C6H8O_Olef_15+OH	2.70E+19	-2.140	5142.9	
!! C3H5-S+O2<=>C2H3CHO+OH				
C*CJCCC*C+O2=>CH2CO+C4H71-4+O	9.86E+25	-3.751	11255.4	
!! C3H5-T+O2<=>CH3COCH2+O				
C*CJCCC*C+O2=>C5H7Or_Olef+CH2O	2.55E+20	-2.608	1565.7	
!! C3H5-T+O2<=>CH3CO+CH2O				
C*CJCCC*C+O2=>C*C*CCC*C+HO2	3.59E+10	-0.270	-413.6	
!! C3H5-T+O2<=>C3H4-A+HO2				

C5H5+HO2=HOOCy (CC*CC*C)	8.39E10	0.600	-2105.6
HOOCy (CC*CC*C) =>C5H5O+OH	1.59E20	-1.500	42857.5

! HHC

H+C*CCCC*CC=C*CCC*CCJC+H2	8.30E+06	2.18	3400
H+C*CCCC*CC=C*CCJCC*CC+H2	8.30E+06	2.18	3400
H+C*CCCC*CC=C*CCCCJC*C+H2	8.30E+06	2.18	3400
!H+C*CCCC*CC=H2+C*CCC*CCJC	1.30E14	0.000	7074.4
!H+C*CCCC*CC=H2+C*CCCCJC*C	7.28E13	0.000	9177.6
!H+C*CCCC*CC=H2+C*CCJCC*CC	1.30E14	0.000	7074.4
CH3+C*CCCC*CC=C*CCC*CCJC+CH4	9.60E+01	3.23	5500
CH3+C*CCCC*CC=C*CCJCC*CC+CH4	9.60E+01	3.23	5500
CH3+C*CCCC*CC=C*CCCCJC*C+CH4	9.60E+01	3.23	5500
!CH3+C*CCCC*CC=CH4+C*CCC*CCJC	1.66E13	0.000	12165.1
!CH3+C*CCCC*CC=CH4+C*CCCCJC*C	7.68E12	0.000	13838.1
!CH3+C*CCCC*CC=CH4+C*CCJCC*CC	1.66E13	0.000	12165.1
C3H5-A+C*CCCC*CC=C*CCC*CCJC+C3H6	2.80E+01	3.61	12700
C3H5-A+C*CCCC*CC=C*CCJCC*CC+C3H6	2.80E+01	3.61	12700
C3H5-A+C*CCCC*CC=C*CCCCJC*C+C3H6	2.80E+01	3.61	12700
!C3H5-A+C*CCCC*CC=C3H6+C*CCC*CCJC	3.58E13	0.000	24425.8
!C3H5-A+C*CCCC*CC=C3H6+C*CCCCJC*C	1.66E13	0.000	26098.8
!C3H5-A+C*CCCC*CC=C3H6+C*CCJCC*CC	3.58E13	0.000	24425.8

H+C*CC (C) CC*C=H2+C7H11r_olef	8.30E+06	2.18	3400
H+C*CC (C) CC*C=H2+C7H11r_olef_2	8.30E+06	2.18	3400
!H+C*CC (C) CC*C=H2+C7H11r_olef	4.72E13	0.000	5903.3
H+C*CC (C) CC*C=H2+C7H11r_olef_23	3.36E14	0.000	12595.3
!H+C*CC (C) CC*C=H2+C7H11r_olef_2	1.52E14	0.000	7170.0
CH3+C*CC (C) CC*C=CH4+C7H11r_olef	9.60E+01	3.23	5500
CH3+C*CC (C) CC*C=CH4+C7H11r_olef_2	9.60E+01	3.23	5500
!CH3+C*CC (C) CC*C=CH4+C7H11r_olef	5.50E12	0.000	10707.2
CH3+C*CC (C) CC*C=CH4+C7H11r_olef_23	3.10E13	0.000	17686.0
!CH3+C*CC (C) CC*C=CH4+C7H11r_olef_2	1.66E13	0.000	12165.1
C3H5-A+C*CC (C) CC*C=C3H6+C7H11r_olef	2.80E+01	3.61	12700
C3H5-A+C*CC (C) CC*C=C3H6+C7H11r_olef_2	2.80E+01	3.61	12700
!C3H5-A+C*CC (C) CC*C=C3H6+C7H11r_olef	1.19E13	0.000	22967.9
C3H5-A+C*CC (C) CC*C=C3H6+C7H11r_olef_23	5.52E13	0.000	29946.7
!C3H5-A+C*CC (C) CC*C=C3H6+C7H11r_olef_2	3.58E13	0.000	24425.8

cy (C*CCCC) =C2H4+C4H6	1.50E+15	0.000	66900
C4H71-3+CH3=CC*CCC	1.00E+13	0.000	0.000
C3H5-A+C2H5=C*CCCC	1.00E+13	0.000	0.000
C3H5-A+C2H3=C*CCC*C	1.00E+13	0.000	0.000
C3H5-A+C4H71-3=C*CCCC*CC	1.00E+13	0.000	0.000
C3H5-A+C4H71-3=C*CC (C) CC*C	1.00E+13	0.000	0.000
C3H5-A+IC4H7=C*C (C) CCC*C	1.00E+13	0.000	0.000
C3H5-A+OH=C3H5OH	2.50E+13	0.000	0.000
C5H5+C3H5-A=C*CCcyCC*CC*C	8.34E+15	-0.700	-500
C5H5+C2H5=CCcyCC*CC*C	8.34E+15	-0.700	-500
C*CC*CCJ+CH3=C6H10_olef_1	1.00E+13	0.000	0.000
C*CC*CCJ+H=C*CC*CC	1.00E+14	0.000	0.000
C*CC*CCJ+H=C*CCC*C	1.00E+14	0.000	0.000
CJcy (CC*CC*C) +CH3=CCcyCC*CC*C	1.00E+13	0.000	0.000
C*cy (CCJC*CC) +CH3=CCcyC*CC*CC	1.00E+13	0.000	0.000
C*cy (CCJCC*C) +CH3=CCcyC*CCC*C	1.00E+13	0.000	0.000
C5H5+C5H5=C10H10	5.00E+13	0.000	0.000

C5H5+C2H3=C*ccyCC*CC*C	8.34E+15	-0.700	-500
C5H5+C3H3=C#CCcyCC*CC*C	8.34E+15	-0.700	-500
C5H5+C3H3=C*C*ccyCC*CC*C	8.34E+15	-0.700	-500
C*C*ccyCC*CC*C=C*CC*cyCC*CC*C	2.72E+38	-7.560	63535
C*CC*cyCC*CC*C+H=C6H5C2H3+H	2.723E+38	-6.654	22277
C7H7+CH3=C6H5CC	1.00E+13	0.000	0.000
C7H7+C2H5=C6H5CCC	1.00E+13	0.000	0.000
C7H7+C2H3=C6H5CC*C	1.00E+13	0.000	0.000
C7H7+C3H5-A=C6H5CCC*C	1.00E+13	0.000	0.000

C6H5CJC*C=>C6H5CJC*C-cy	4.20E+11	0.267	33485
C6H5CJC*C-cy=>C6H5CJC*C	1.70E+12	0.426	25789
C6H5CJC*C-cy=>C9H8+H	1.80E+09	1.300	27400
C6H5CJC*CC=>C6H5CJC*CC-cy	4.80E+10	0.474	28944
DUP			
C6H5CJC*CC-cy=>C6H5CJC*CC	1.90E+13	0.135	23996
DUP			
C6H5CJC*CC=>C6H5CJC*CC-cy	4.90E+10	0.473	28967
DUP			
C6H5CJC*CC-cy=>C6H5CJC*CC	1.50E+13	0.138	24402
DUP			
C6H5CJC*CC-cy=>M1H1Indene+H	1.80E+09	1.300	27400
C6H5CCJC*C=>C6H5CCJC*C-cy	3.40E+08	0.805	20698
C6H5CCJC*C-cy=>C6H5CCJC*C	1.30E+12	0.412	19168
C6H5CCJC*C-cy=>C10H8+H2+H	1.80E+09	1.300	27400
C6H5CCCCJ=>C6H5CCCCJ-cy	1.10E+06	1.136	7815
C6H5CCCCJ-cy=>C6H5CCCCJ	2.00E+12	0.410	22323
C6H5CCCCJ-cy=>C10H8+H+H2+H2	1.80E+09	1.300	27400
C6H5CCCJC=>C6H5CCCJC-cy	1.10E+08	1.018	14938
C6H5CCCJC-cy=>C6H5CCCJC	3.10E+12	0.369	22036
C6H5CCCJC=>M1H1Indene+H+H2	1.80E+09	1.300	27400
C6H5CCCJ=>C6H5CCCJ-cy	1.10E+08	1.018	14938
C6H5CCCJ-cy=>C6H5CCCJ	3.10E+12	0.369	22036
C6H5CCCJ=>C9H8+H+H2	1.80E+09	1.300	27400

! Serinyel et al. - An experimental and modeling study of the low- and high-temperature oxidation of cyclohexane

cy (CJCCCC) +O2=cy (C*CCCC) +HO2	7.90E+12	0.000	5000.
cy (CJCCCC) +O2=JOOcy (CCCCC)	1.80E+19	-2.500	0.0
JOOcy (CCCCC) =>cy (C*CCCC) +HO2	8.50E+12	0.000	32100.
JOOcy (CCCCC) =HOOcy (CJCCCC)	1.05E+09	1.355	38850.0
HOOcy (CJCCCC) =>OH+O*cy (CCCCC)	1.00E+09	0.000	7500.0
JOOcy (CCCCC) =HOOcy (CCCCJCC)	1.05E+07	1.739	30250.0
HOOcy (CCCCJCC) =>OH+epoxy14cy6	4.20E+09	0.935	16400.0
JOOcy (CCCCC) =HOOcy (CCJCCCC)	3.63E+08	1.401	31740.0
HOOcy (CCJCCCC) =>OH+epoxy12cy6	4.90E+10	0.564	10250.0
HOOcy (CCJCCCC) =>HO2+cy (C*CCCC)	8.50E+12	0.000	26000.0
JOOcy (CCCCC) =HOOcy (CCCJCCC)	1.82E+07	1.668	25100.0
HOOcy (CCCJCCC) =>OH+C*CCCC*O	3.30E+12	0.248	20440.0

JOOcy (CCC*CCC) =HOOcy (CCC*CCJC)	1.82E+07	1.668	22600.0	! RDB (-
2500 cal/mol - EXGAS)				
HOOcy (CCC*CCJC) =>OH+C*CC*CCC*O	3.30E+12	0.248	20440.0	

C*CC*CCC*O=CO+C*CC*CC	7.31E+05	1.676	34760
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HocyCCCC (OOJ) CC=HocyCCJCCPCC	1.82E+07	1.668	25100.0
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HOcyCCJCCPCC=>OH+C*CC(OH)CCC*O    3.30E+12    0.248    20440.0

!C5H7+O2=C5H6+HO2                    5.2E11                0.0                2500                !
TOUCHARD05
!C*cy(CCJCC*C)+O2=fulvene+HO2         5.2E11                0.0                2500
!C*cy(CCJC*CC)+O2=fulvene+HO2         5.2E11                0.0                2500
!Ccy(CJC*CC*C)+O2=fulvene+HO2        5.2E11                0.0                2500

! Mendes et al. - hydrogen abstraction from aldehydes
C*CC*CCC*O+OH=C*CC*CCCJ*O+H2O        61329.9               2.650              -4586.4
C*CC*CCC*O+H=C*CC*CCCJ*O+H2          8.66E5                2.300              1426
C*CC*CCC*O+HO2=C*CC*CCCJ*O+H2O2      1.01E-4               5.000              3429
C*CC*CCC*O+CH3=C*CC*CCCJ*O+CH4       3.94                  3.600              4223
C*CC*CCCJ*O=>C*CC*CCJ+CO              3.30E12               0.620              17298.8

! Mendes et al. - hydrogen abstraction from aldehydes
! C2H3CHO+OH=C2H3CO+H2O                61329.9               2.650              -4586.4
C2H3CHO+OH<=>C2H3CO+H2O                3.370E+012            0.000
-619.0
C2H3CHO+H=C2H3CO+H2                    8.66E5                2.300              1426
C2H3CHO+HO2=C2H3CO+H2O2                1.01E-4               5.000              3429
C2H3CHO+CH3=C2H3CO+CH4                 3.94                  3.600              4223

C2H3CHO+OH=>C2H3OH+HCO 1.56E+08        1.29                 -2652.9
DUP
C2H3CHO+OH=>C2H3OH+HCO 2.38E+05        2.18                 1063
DUP

! Source: CBS-QB3 HHC - unpublished - part of the calculations are
already included in the C3H5O PES by Goldsmith
!H+C2H3CHO=CH2CH2CHO 1.90E+09          1.43                 2300
H+C2H3CHO=CH3CHCHO  5.80E+09          1.40                 200
!CH2CH2CHO=C2H5CO   4.30E+05          1.95                 30400
!CH2CH2CHO=C2H4+HCO 3.00E+10          0.90                 22200
CH3CHCHO=CH2CH2CHO  1.50E+08          1.55                 38800
CH3CHCHO=C2H5CO     1.50E+10          1.00                 40800
CH3CHCHO=H+CH3CHCO  7.40E+10          1.05                 48600
!C2H5CO=C2H5+CO     1.20E+13          0.34                 15300
!C2H5CO=CH3+CH2CO   9.10E+09          1.21                 40200
!C2H5CO=H+CH3CHCO  1.20E+09          1.42                 45800

! Source: Kun & CBS-QB3 HHC - unpublished
C5H6+H=C5H5+H2      6.50E+07  1.87  2900
C5H6+CH3=C5H5+CH4   1.60E+03  2.88  4300
C5H6+C3H5-A=C5H5+C3H6 1.91E+02  3.14  11500
O2+C5H6=HO2+C5H5    2.00E13  0.000  30799.8

! C4H7 mechanism - Source: CBS-QB3 HHC - unpublished
C4H71-4=C2H4+C2H3   1.20E+11  0.83  35000  ! RDB /2
C4H71-4=C4H6+H      3.10E+06  2.05  30600
C4H71-4=C4H71-3     1.60E+06  2.05  26700
C4H71-3=H+C4H6      7.00E+07  1.87  45900
C4H71-4=C4H71-1     3.40E+06  1.54  23700
C4H71-1=C2H2+C2H5   1.40E+13  0.56  32100

! C6H6 mechanism - Hansen et al.
C3H3+C3H3<=>C6H5+H   2.020E+033  -6.050  15940.0
C3H3+C3H3<=>C6H6     1.640E+066  -15.902  27529.0

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```

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
fulvene=C6H6          5.62E+81  -19.40   121500
fulvene+H=C6H6+H     3.00E+12    0.50   2000

! C5H7
C3H5-A+C2H2 <=> CJ*CCC*C      4.88E+12   -1.52   2644.8 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 9.2E+00%
! Collider = !N2
! AvgAbsErr: 4.8% MaxAbsErr: 13.1%
!C3H5-A+C2H2 <=> C#CCC*C+H  1.60E+04    2.14  25608.9 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 1.2E+01%
! Collider = !N2
! AvgAbsErr: 20.9% MaxAbsErr: 78.3%
C3H5-A+C2H2 <=> cy(C*CCCJC)  5.38E+59  -15.04  28079.2 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 5.4E+00%
! Collider = !N2
! AvgAbsErr: 4.9% MaxAbsErr: 14.4%
C3H5-A+C2H2 <=> C5H6+H  1.76E+33   -6.42  24524.7 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 3.1E+00%
! Collider = !N2
! AvgAbsErr: 3.1% MaxAbsErr: 14.0%
!CJ*CCC*C <=> C#CCC*C+H      7.97E+13   -1.58  10753.9 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 9.2E+00%
! Collider = !N2
! AvgAbsErr: 4.9% MaxAbsErr: 13.3%
CJ*CCC*C <=> cy(C*CCCJC)     2.72E+59  -15.25  27550.6 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 5.2E+00%
! Collider = !N2
! AvgAbsErr: 3.4% MaxAbsErr: 9.2%
CJ*CCC*C <=> C5H6+H      7.77E+31   -6.54  23113.4 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 1.1E+00%
! Collider = !N2
! AvgAbsErr: 3.3% MaxAbsErr: 12.1%
!cy(C*CCCJC) <=> C#CCC*C+H  4.89E+64  -15.42  69755.8 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 5.0E+00%
! Collider = !N2
! AvgAbsErr: 5.4% MaxAbsErr: 14.1%
cy(C*CCCJC) <=> C5H6+H  2.59E+43   -9.39  47662.0 ! 1.00E+00 ATM,
Tffit: 5.00E+02- 1.50E+03K, Avg ERR= 6.4E+00%
! Collider = !N2
! AvgAbsErr: 5.9% MaxAbsErr: 15.7%
C*CC*CCJ=>C5H7          7.48E10      0.000  21988.0
!CJ*CCC*C=C2H2+C3H5-A  1.55E14      0.000  26218.3
!CJ*CCC*C=cy(C*CCCJC)  3.74E10      0.000  14507.3
!C5H6+H=cy(C*CCCJC)    1.64E14      0.000  5377.5

! C5H9 mechanism
! Source: Reactions of allylic radicals that impact molecular weight
growth kinetics - Wang et al. (2015)
C3H5-A+C2H4=>C*CCCCJ  2.13E+12    0.000  14700
C*CCCCJ=>C*CCC*C+H    1.44E+13    0.000  36900
!C*CCCCJ=>CJcy(CCCC)  7.67E+10    0.000  16400

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!CJcy(CCCC)=>C*cy(CCCC)+H 3.00E+14 0.000 38700
C*CCCCJ=>cy(CJCCCC) 7.69E+10 0.000 15400
cy(CJCCCC)=>cy(C*CCCC)+H 4.41E+14 0.000 36100
C*CCCCJ=>C*CCJCC 1.62E+12 0.000 32200
C*CCJCC=>C*CC*CC+H 1.62E+14 0.000 46600
C*CCJCC=>C4H6+CH3 6.16E+14 0.000 38000
C*CCCCJ=>C*CCCJC 9.01E+12 0.000 38100
C*CCCJC=>C*CCC*C+H 2.38E+13 0.000 39200
C*CCCJC=>C*CC*CC+H 1.45E+13 0.000 33900
C*CCCCJ=>C3H5-A+C2H4 1.48E+13 0.000 20700
C*CCC*C+H=>C*CCCCJ 9.74E+13 0.000 3660
!CJcy(CCCC)=>C*CCCCJ 3.28E+13 0.000 14300
!C*cy(CCCC)+H=>CJcy(CCCC) 1.30E+13 0.000 1600
!cy(CJCCCC)=>C*CCCCJ 1.70E+14 0.000 34500 ! RDB
!cy(C*CCCC)+H=>cy(CJCCCC) 1.78E+14 0.000 2180 ! RDB
C*CCJCC=>C*CCCCJ 1.27E+13 0.000 49600
C*CC*CC+H=>C*CCJCC 1.02E+14 0.000 3020
C4H6+CH3=>C*CCJCC 5.82E+12 0.000 5440
C*CCCJC=>C*CCCCJ 1.10E+13 0.000 41300
C*CCC*C+H=>C*CCCJC 2.60E+13 0.000 1560
C*CC*CC+H=>C*CCCJC 5.84E+13 0.000 4390
!C*CCCCJ=cy(CJCCCC) 7.48E10 0.000 17662.1
!C*CCCCJ=C3H5-A+C2H4 1.51E13 0.000 20745.2
!C*CC*CC+H=C*CCCJC 8.20E13 0.000 5377.5
!C*CCC*C+H=C*CCCCJ 1.29E14 0.000 5377.5
!C*CC*CC+H=C*CCJCC 6.11E13 0.000 3704.5
!C*CCC*C+H=C*CCCJC 1.11E14 0.000 3847.9
!cy(C*CCCC)+H=cy(CJCCCC) 1.35E14 0.000 4803.9
!C*CCJCC=C4H6+CH3 2.39E14 0.000 39458.9
! Tsang
C*CC(CJ)C=C4H6+CH3 4.27E+11 0.42 30617
C*CC(CJ)C=C*CCCJC 1.66E+10 1.135 11711

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! C5H8 + R

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C3H5-A+cy(C*CCCC)=C3H6+C5H7 1.33E+02 3.26 12800
CH3+cy(C*CCCC)=CH4+C5H7 1718 2.95 5320

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! C6H7

! Source: unpublished - Sharma and Merchant (2014)

```

fulvene+H=Ccy(CJC*CC*C) 1.70E+09 1.46 -700
fulvene+H=CJcy(CC*CC*C) 1.30E+08 1.76 2000
fulvene+H=C*cy(CCJC*CC) 7.30E+09 1.48 400
fulvene+H=C*cy(CCJCC*C) 3.50E+09 1.52 900
Ccy(CJC*CC*C)=CJcy(CC*CC*C) 2.20E-03 4.91 40400
CJcy(CC*CC*C)=C*cy(CCJC*CC) 2.20E+07 1.54 13400
C*cy(CCJC*CC)=C*cy(CCJCC*C) 9.20E+03 2.81 30200
CJcy(CC*CC*C)=cy(CJC*CcyCCC) 3.20E+11 0.17 4400
cy(CJC*CcyCCC)=cy(C*CC*CCJC) 8.50E+11 0.41 16700
cy(C*CC*CCJC)=C6H6+H 1.80E+09 1.3 27400

```

! Source: The Reaction of n- and i-C4H5 Radicals with Acetylene

```

C4H5-N+C2H2=H+C6H6 1.39E+16 -1.000 8895
C4H5-N+C2H2=H+fulvene 4.62E+15 -0.890 9138
C4H5-I+C2H2=H+C6H6 1.67E+23 -3.300 24946
C4H5-I+C2H2=H+fulvene 6.80E+24 -3.450 20327

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! Herbinet

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C4H4+C2H3=C6H6+H 1.90E+12 0.000 2.50E+03

```

! C6H8 mechanism C3H5-A + C3H3 - Miller et al. (2010)

!C3H5-A+C3H3=fulvene+2H	3.26E+29	-5.40	3390
C3H5-A+C3H3=C#CCCC*C	3.62E+56	-12.78	23846.0
C3H5-A+C3H3=C*C*CCC*C	3.27E+55	-12.42	24912.0
C3H5-A+C3H3=C*cy (CCJCC*C) +H	1.88E+38	-7.526	23878.0
C#CCCC*C=C*C*CCC*C	1.25E+32	-6.242	45805.0
C#CCCC*C=C*cy (CCJCC*C) +H	3.20E+32	-6.314	51585.0
C*C*CCC*C=C*cy (CCJCC*C) +H	4.34E+83	-20.57	102400.0

! C6H8 mechanism - Sharma and Green (2009)

Ccy (CC*CC*C)=Ccy (C*CC*CC)	7.03E+08	1.200	24800
Ccy (C*CC*CC)=Ccy (C*CCC*C)	1.65E+07	2.100	25100
C5H5+CH3=Ccy (CC*CC*C)	8.34E+15	-0.700	-500
fulvene+H2=Ccy (CC*CC*C)	1.44E+05	3.900	81100
fulvene+H2=Ccy (C*CC*CC)	6.08E+07	1.400	71000
fulvene+H2=Ccy (C*CCC*C)	1.62E+06	1.600	55500
Ccy (CJC*CC*C) +H=Ccy (CC*CC*C)	4.57E+14	-0.100	400
Ccy (CJC*CC*C) +H=Ccy (C*CC*CC)	4.09E+13	0.300	100
C*cy (CCJC*CC) +H=Ccy (C*CC*CC)	1.05E+12	0.600	-200
Ccy (CJC*CC*C) +H=Ccy (C*CCC*C)	9.05E+13	0.100	0
C*cy (CCJCC*C) +H=Ccy (C*CCC*C)	3.43E+12	0.500	-100
CJcy (CC*CC*C) +H=Ccy (CC*CC*C)	2.10E+12	0.600	-800
C*CC*CC*C=>cy (C*CC*CCC)	4.50E+12	0.000	43259
!cy (C*CCC*CC)=C6H6+H2	2.30E+12	0.000	43737
!cy (C*CC*CCC)=C6H6+H2	2.50E+13	0.000	59033

fulvene+HO2=C*cy (CCJCC*C) +O2	1.300E+015	-1.070	9530.0	!
C5H6+HO2<=>C5H7+O2				
fulvene+HO2=C*cy (CCJC*CC) +O2	1.300E+015	-1.070	9530.0	!
C5H6+HO2<=>C5H7+O2				

! C6H8 + R

!H+cy (C*CC*CCC)=cy (C*CC*CCJC) +H2	6.60E+08	1.700	2500	! HHC
H+cy (C*CC*CCC)=H2+cy (C*CC*CCJC)		2.60E14	0.000	
	7074.4			
!CH3+cy (C*CC*CCC)=CH4+cy (C*CC*CCJC)	2.90E+03	2.890	3400	! HHC
CH3+cy (C*CC*CCC)=CH4+cy (C*CC*CCJC)	3.31E+13	0.000	12165.1	
!C3H5-A+cy (C*CC*CCC)=C3H6+cy (C*CC*CCJC)	1.88E+02	3.180	9860	! Kun
C3H5-A+cy (C*CC*CCC)=C3H6+cy (C*CC*CCJC)		7.15E13	0.000	
	24425.8			
!H+cy (C*CCC*CC)=cy (C*CC*CCJC) +H2	5.20E+08	1.710	1900	! HHC
H+cy (C*CCC*CC)=H2+cy (C*CC*CCJC)		4.03E14	0.000	
	6190.1			
!CH3+cy (C*CCC*CC)=cy (C*CC*CCJC) +CH4	2.80E+03	2.890	3500	! HHC
CH3+cy (C*CCC*CC)=CH4+cy (C*CC*CCJC)	3.57E+13	0.000	9918.5	
!C3H5-A+cy (C*CCC*CC)=C3H6+cy (C*CC*CCJC)	3.89E+02	3.120	9480	! Kun
C3H5-A+cy (C*CCC*CC)=C3H6+cy (C*CC*CCJC)		7.70E13	0.000	
	22179.2			
H+Ccy (C*CC*CC)=Ccy (CJC*CC*C) +H2	5.70E+07	1.890	3000	
H+Ccy (C*CC*CC)=H2+C*cy (CCJC*CC)	2.70E+06	2.270	2800	
CH3+Ccy (C*CC*CC)=CH4+Ccy (CJC*CC*C)	9.40E+02	2.880	4000	
CH3+Ccy (C*CC*CC)=CH4+C*cy (CCJC*CC)	5.10E+01	3.310	5300	
H+Ccy (C*CCC*C)=Ccy (CJC*CC*C) +H2	6.50E+07	1.870	2900	
H+Ccy (C*CCC*C)=H2+C*cy (CCJCC*C)	1.50E+06	2.340	3800	
CH3+Ccy (C*CCC*C)=CH4+Ccy (CJC*CC*C)	1.60E+03	2.880	4300	
CH3+Ccy (C*CCC*C)=CH4+C*cy (CCJCC*C)	5.50E+01	3.290	620	
H+Ccy (CC*CC*C)=Ccy (CJC*CC*C) +H2	1.30E+08	1.730	2500	

H+Ccy (CC*CC*C)=H2+CJcy (CC*CC*C)	2.30E+07	2.040 7200
CH3+Ccy (CC*CC*C)=CH4+Ccy (CJC*CC*C)	1.50E+03	2.800 2600
CH3+Ccy (CC*CC*C)=CH4+CJcy (CC*CC*C)	8.70E+02	2.960 9500

! C6H9 mechanism

! Source: Reactions of allylic radicals that impact molecular weight growth kinetics - Wang et al. (2015)

C*CCJC*CC=>C6H9-A	1.32E+13	0	44800
cy (C*CCCJCC) =>C6H9-A	5.03E+13	0	28800
CJcy (CCC*CC) =>C6H9-A	4.68E+13	0	23400
C6H9-A=>C4H6+C2H3	1.71E+15	0	45100
Ccy (CCJC*CC) =>C*CCJC*CC	5.30E+13	0	43200
cy (C*CCC*CC) +H=>cy (C*CCCJCC)	4.15E+14	0	3710
cy (C*CC*CCC) +H=>cy (C*CCCJCC)	1.32E+14	0	3330
Ccy (CCJC*CC) =>CJcy (CCC*CC)	8.28E+12	0	48100
C*cy (CCC*CC) +H=>CJcy (CCC*CC)	2.47E+13	0	4940
CH3+C5H6=>Ccy (CCJC*CC)	1.50E+13	0	6830
Ccy (CC*CC*C) +H=>Ccy (CCJC*CC)	2.60E+13	0	2160
Ccy (C*CC*CC) +H=>Ccy (CCJC*CC)	2.60E+13	0	2160
C6H9-A=>C*CCJC*CC	1.84E+12	0	31300
C6H9-A=>cy (C*CCCJCC)	1.10E+11	0	21100
C6H9-A=>CJcy (CCC*CC)	4.29E+11	0	20900
C4H6+C2H3=>C6H9-A	1.38E+13	0	2310
C*CCJC*CC=>Ccy (CCJC*CC)	2.45E+12	0	36600
cy (C*CCCJCC) =>cy (C*CCC*CC) +H	2.01E+14	0	35000
cy (C*CCCJCC) =>cy (C*CC*CCC) +H	8.94E+13	0	34600
CJcy (CCC*CC) =>Ccy (CCJC*CC)	5.84E+12	0	30500
CJcy (CCC*CC) =>C*cy (CCC*CC) +H	2.85E+13	0	35900
Ccy (CCJC*CC) =>CH3+C5H6	9.89E+14	0	38900
Ccy (CCJC*CC) =>Ccy (CC*CC*C) +H	4.95E+12	0	46400
Ccy (CCJC*CC) =>Ccy (C*CC*CC) +H	1.54E+13	0	43000

! Source: Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene - Buras et al. (2015)

!C4H6+C2H3=C6H9-A	3.91E+04	2.404 420
!C6H9-A=H+C*CC*CC*C	2.29E+06	2.017 40664
!C6H9-A=cy (C*CCCJCC)	5.04E+08	0.700 20246
!C6H9-A=CJcy (CCC*CC)	5.25E+08	0.846 19298
!CJcy (CCC*CC) =C*cy (CCC*CC) +H	1.97E+07	1.802 32304
!cy (C*CCCJCC) =cy (C*CC*CCC) +H	7.49E+08	1.395 33132
!cy (C*CCCJCC) =cy (C*CCC*CC) +H	2.10E+09	1.299 33394
!CJcy (CCC*CC) =C6H9r_R5_2	5.27E-07	5.639 24541
!CJcy (CCC*CC) =Ccy (CCJC*CC)	3.54E-16	8.138 14583
!Ccy (CCJC*CC) =CH3+C5H6	4.96E+11	0.717 38962
!C6H9r_R5_2=Ccy (CCJC*CC)	3.24E-08	6.224 24481
! Source: Genesys		
!C*CC*CC*C+H=C6H9-A	1.49E14	0.000 4278.1
!C6H9-A=cy (C*CCCJCC)	5.22E9	0.000 17423.1
!C6H9-A=C*CCJC*CC	3.00E11	0.000 29875.0
!C6H9-A=CJcy (CCC*CC)	2.80E10	0.000 16855.2
!C6H9-A=C4H6+C2H3	2.35E14	0.000 45290.5
!C*CCJC*CC=Ccy (CCJC*CC)	3.74E10	0.000 21892.4
!CJcy (CCC*CC) =Ccy (CCJC*CC)	4.80E12	0.000 36590.9
!cy (C*CCC*CC) +H=cy (C*CCCJCC)	2.70E14	0.000 4803.9
!cy (C*CC*CCC) +H=cy (C*CCCJCC)	1.64E14	0.000 5377.5
!C*cy (CCC*CC) +H=CJcy (CCC*CC)	3.42E13	0.000 6190.1
!Ccy (CCJC*CC) =CH3+C5H6	2.61E14	0.000 39363.3
!Ccy (CC*CC*C) +H=Ccy (CCJC*CC)	1.22E14	0.000 3704.5

!DUP
!Ccy(CC*CC*C)+H=Ccy(CCJC*CC) 1.22E14 0.000 3704.5
!DUP
!Ccy(C*CC*CC)+H=Ccy(CCJC*CC) 1.62E13 0.000 4517.1

! C7H7

! Source: Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions - da Silva (2010)

! Note: Irreversible reactions given the lack of thermodynamic data

C5H5+C2H2=>C7H7_3 4.08E+05 2.240 10800
C7H7_3=>C7H7_4 9.25E+11 0.160 9810
C7H7_4=>cC7H7 4.51E+12 0.260 25250
cC7H7=>C7H7_6 5.50E+08 1.560 62120
C7H7_6=>C7H7_7 2.48E+06 1.850 26830
C7H7_7=>C7H7_8 2.10E+12 0.140 300
C7H7_8=>C7H7 1.24E+12 0.310 3620
C7H7=>C7H7_10 1.98E+12 0.500 61000
C7H7_10=>C7H7_14 2.80E+13 0.150 19350
C7H7_3=>C7H7_11 1.01E+10 0.970 19170
C7H7_11=>C#Ccy(C*CC*CC)+H 4.06E+10 1.160 26180
C7H7_11=>C7H7_13 7.42E+04 2.230 10590
C7H7_13=>C7H7_14 1.17E+04 2.780 62710
C7H7_14=>C7H7_15 6.21E+08 1.380 15290
C7H7_13=>fulvenallene+H 4.16E+10 1.240 65980
C7H7_15=>fulvenallene+H 1.02E+13 0.340 46700
C7H7_3=>C5H5+C2H2 2.36E+12 0.630 17860
C7H7_4=>C7H7_3 6.35E+12 0.340 26730
cC7H7=>C7H7_4 1.72E+12 0.680 53730
C7H7_6=>cC7H7 1.37E+08 1.360 25060
C7H7_7=>C7H7_6 1.47E+06 1.900 21050
C7H7_8=>C7H7_7 7.85E+12 -0.010 6880
C7H7=>C7H7_8 3.45E+12 0.250 55690
C7H7_10=>C7H7 4.52E+12 0.190 10050
C7H7_14=>C7H7_10 1.69E+11 0.590 11210
C7H7_11=>C7H7_3 5.61E+10 0.810 16280
C#Ccy(C*CC*CC)+H=>C7H7_11 4.14E+08 1.500 2760
C7H7_13=>C7H7_11 2.80E+04 2.390 54810
C7H7_14=>C7H7_13 1.17E+03 3.070 23500
C7H7_15=>C7H7_14 1.98E+10 0.940 36350
fulvenallene+H=>C7H7_13 3.10E+09 1.510 600
fulvenallene+H=>C7H7_15 1.27E+11 0.850 -73

! C7H8 mechanism - Oehlschlaeger et al. (2007)

C7H8=H+C7H7 2.09E+15 0.000 87510
C7H8=C6H5+CH3 2.66E+16 0.000 97880

! C7H9 mechanism

C7H8+H=C6H6+CH3 5.78E+13 0.000 8088
Ccy(C*CCCJC*C)=C7H8+H 1.80E+09 1.300 27400
Ccy(CJCC*CC*C)=C7H8+H 1.80E+09 1.300 27400
Ccy(CCJC*CC*C)=C7H8+H 1.80E+09 1.300 27400
Ccy(C*CCJCC*C)=C7H8+H 1.80E+09 1.300 27400

! C7H9 mechanism - Vandeputte et al.

CCcyCJC*CC*C=fulvene+CH3 1.06E+11 1.15 39700
CJCcyCC*CC*C=CCcyCJC*CC*C 9.37E+06 1.60 25100
CJCcyCC*CC*C=C5H5+C2H4 1.87E+11 0.68 13900


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! C7H10 mechnaism
! cy(C*CC*CCJC)+CH3=Ccy(CC*CC*CC) 1.00E+13 0.00 0.00
! cy(C*CC*CCJC)+CH3=Ccy(CC*CCC*C) 1.00E+13 0.00 0.00
!Ccy(CC*CCC*C)=C7H8+H2 2.30E+12 0.000 43737
!Ccy(C*CCCC*C)=C7H8+H2 2.50E+13 0.000 59033
!Ccy(CC*CC*CC)=C7H8+H2 2.50E+13 0.000 59033
!Ccy(C*CCC*CC)=C7H8+H2 2.30E+12 0.000 43737
!Ccy(C*CC*CCC)=C7H8+H2 2.50E+13 0.000 59033
C*CC*CC*CC=Ccy(CC*CC*CC) 4.50E+12 0.000 43259
C*CC*CCC*C=Ccy(CC*CC*CC) 4.50E+12 0.000 43259

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! C7H11 mechanism

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! Source: Reactions of allylic radicals that impact molecular weight
growth kinetics - Wang et al. (2015)

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C3H5-A+C4H6=>C*CCCCJC*C 1.76E+12 0.000 11060
C*CCCCJC*C=>C*CCJCC*CC 5.41E+11 0.000 24010
C*CCJCC*CC=>Ccy(CCJCC*CC) 1.04E+11 0.000 21250
Ccy(CCJCC*CC)=>cy(C*CCC*CC)+CH3 5.44E+14 0.000 30250
C*CCJCC*CC=>CC*CC*CCJC 1.77E+12 0.000 31150
CC*CC*CCJC=>C7H11r_R5_73 1.78E+12 0.000 35630
C7H11r_R5_73=>Ccy(CC*CC*C)+CH3 1.95E+15 0.000 40000
C*CCCCJC*C=>C*CCC*CCJC 3.77E+12 0.000 35950
C*CCC*CCJC=>CCC*CC*CCJ 5.25E+12 0.000 31690
CCC*CC*CCJ=>C7H11r_R5_75 2.33E+12 0.000 36950
C7H11r_R5_75=>C5H6+C2H5 3.02E+14 0.000 36990
C*CCC*CCJC=>Ccy(CC*CCCJC) 1.33E+11 0.000 22060
Ccy(CC*CCCJC)=>H+Ccy(C*CCC*CC) 8.11E+13 0.000 34830
Ccy(CC*CCCJC)=>H+Ccy(CC*CC*CC) 8.14E+13 0.000 34790
C*CCCCJC*C=>cy(CJCCC*CCC) 7.75E+09 0.000 23170
cy(CJCCC*CCC)=>cy(C*CCC*CCC)+H 2.44E+14 0.000 38230
C*CCCCJC*C=>C7H11r_R5_19 4.94E+10 0.000 23490
C7H11r_R5_19=>C*Ccy(CCC*CC)+H 2.51E+14 0.000 36800
C7H11r_R5_19=>C7H10_R5_11+H 4.10E+14 0.000 36600
C*CCCCJC*C=>CJcy(CCC*CCC) 1.22E+11 0.000 20320
CJcy(CCC*CCC)=>C*cy(CCC*CCC)+H 1.72E+14 0.000 39960
C*CCCCJC*C=>C3H5-A+C4H6 2.74E+13 0 28110
C*CCJCC*CC=>C*CCCCJC*C 1.13E+12 0 26400
Ccy(CCJCC*CC)=>C*CCJCC*CC 7.54E+13 0 28460
cy(C*CCC*CC)+CH3=>Ccy(CCJCC*CC) 1.32E+13 0 9890
CC*CC*CCJC=>C*CCJCC*CC 1.41E+13 0 44970
C7H11r_R5_73=>CC*CC*CCJC 5.08E+13 0 41100
Ccy(CC*CC*C)+CH3=>C7H11r_R5_73 1.52E+13 0 6680
C*CCC*CCJC=>C*CCCCJC*C 1.34E+13 0 38710
CCC*CC*CCJ=>C*CCC*CCJC 1.38E+13 0 41910
C7H11r_R5_75=>CCC*CC*CCJ 5.64E+13 0 43810
C5H6+C2H5=>C7H11r_R5_75 2.15E+13 0 6780
Ccy(CC*CCCJC)=>C*CCC*CCJC 5.49E+13 0 28720
H+Ccy(C*CCC*CC)=>Ccy(CC*CCCJC) 4.34E+13 0 3120
H+Ccy(CC*CC*CC)=>Ccy(CC*CCCJC) 6.90E+13 0 3280
cy(CJCCC*CCC)=>C*CCCCJC*C 1.68E+13 0 27120
cy(C*CCC*CCC)+H=>cy(CJCCC*CCC) 8.00E+13 0 3500
C7H11r_R5_19=>C*CCCCJC*C 1.92E+13 0 26720
C*Ccy(CCC*CC)+H=>C7H11r_R5_19 1.25E+14 0 3420
C7H10_R5_11+H=>C7H11r_R5_19 1.57E+14 0 2900
CJcy(CCC*CCC)=>C*CCCCJC*C 1.67E+14 0 32590
C*cy(CCC*CCC)+H=>CJcy(CCC*CCC) 2.06E+14 0 3920

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! Source: Genesys

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!C4H6+C3H5-A=C*CCCCJC*C      2.59E12      0.000 13790.3
!C*CCC*CCJC=CCC*CC*CCJ 6.00E11      0.000 31285.1
!C*CCC*CCJC=Ccy (CC*CCCJC)    5.22E9      0.000 17327.5
!C*CCCCJC*C=C*CCC*CCJC 3.00E11      0.000 32121.6
!C*CCCCJC*C=CJcy (CCC*CCC)    1.95E9      0.000 17160.2
!C*cy (CCC*CCC) +H=CJcy (CCC*CCC) 1.71E13      0.000 6190.1
!Ccy (CC*CC*CC) +H=Ccy (CC*CCCJC) 8.20E13      0.000 5377.5
!DUP
!Ccy (CC*CC*CC) +H=Ccy (CC*CCCJC) 8.20E13      0.000 5377.5
!DUP
!CC*CC*CCJC=C*CCJCC*CC 1.80E12      0.000 42924.4
!C*CCCCJC*C=C*CCJCC*CC 3.70E10      0.000 25118.9
!C*CCCCJC*C=C7H11r_R5_19    3.74E10      0.000 24617.0
!CC*CC*CCJC=C7H11r_R5_73    7.48E10      0.000 23398.1
!CCC*CC*CCJ=C7H11r_R5_75    3.74E10      0.000 21892.4
!C*CCJCC*CC=Ccy (CCJCC*CC)   5.22E9      0.000 18928.8
!C*Ccy (CCC*CC) +H=C7H11r_R5_19 1.35E14      0.000 4803.9
!DUP
!C*Ccy (CCC*CC) +H=C7H11r_R5_19 1.35E14      0.000 4803.9
!DUP
!C7H10_R5_11+H=C7H11r_R5_19 6.75E13      0.000 4803.9
!DUP
!C7H10_R5_11+H=C7H11r_R5_19 6.75E13      0.000 4803.9
!DUP
!C7H11r_R5_73=Ccy (CC*CC*C) +CH3 5.22E14      0.000 39363.3
!C7H11r_R5_75=C2H5+C5H6      1.87E14      0.000 37284.0

```

! Benzene submechanism - Herbinet et al. (2013)

```

C6H6+H=C6H5+H2      1.22E+08 2.031 15880
C6H6+O=C6H5+OH      2.00E+13 0.000 14700
C6H6+OH=C6H5+H2O    1.36E+04 2.700 620
C6H6+HO2=C6H5+H2O2  9.20E+12 0.000 28810
C6H6+CH3=C6H5+CH4   2.07E+00 3.861 13300
C6H5+C3H6=C6H6+C3H5-A 7.94E+13 0.000 11940
C6H6+C2H5=C6H5+C2H6  6.30E+11 0.000 15000
C6H6+C2H3=C6H5C2H3+H 7.90E+11 0.000 6400
C6H6+O=C6H5O+H      2.80E+13 0.000 4910
C6H6+OH=C6H5OH+H    1.30E+13 0.000 10600
C4H4+O=C3H4-P+CO    3.00E+13 0.00 1800
C4H4+O=C3H4-A+CO    2.70E+13 0.00 1800

```

! Toluene submechanism - Herbinet et al. (2013)

```

C7H8+O=C7H7+OH      6.3E11 0.0 0.0
C7H8+OH=C7H7+H2O    5.2E09 1.0 0.87E3
C7H8+HO2=C7H7+H2O2  4.0E11 0.0 14.0E3
C7H7+HO2=C6H5CH2OOH  8.21E4 2.20 -5.13E3
C6H5CH2OOH=C6H5CH2O+OH 3.29E13 0.42 39.89E3
C6H5CH2OOH=C6H5CHO+H2O 7.45E8 1.19 46.04E3
C6H5CH2O=H+C6H5CHO   5.26E28 -5.081 22.25E3
C6H5CH2O=C6H6+HCO    2.37E32 -6.095 28.81E3
C6H5CH2O=C6H5+CH2O   7.21E33 -6.21 36.85E3

```

! Benzaldehyde submechnaisme - Herbinet et al. (2013)

```

C6H5CHO+H=C6H6+HCO   5.8E13 0.0 8.1E3
C6H5CHO+H=C6H5CO+H2  4.0E13 0.0 3.2E3
C6H5CHO+O=C6H5CO+OH  6.0E12 0.0 1.8E3
C6H5CHO+OH=C6H5CO+H2O 7.8E12 0.0 0.0
C6H5CHO+HO2=C6H5CO+H2O2 3.0E12 0.0 11.0E3

```

C6H5CHO+CH3=C6H5CO+CH4 2.0E-6 5.6 2.5E3
 C6H5CO=C6H5+CO 4E14 0.0 29.5e3

! Ethylbenzene submechanism - Herbinet et al. (2013)
 C6H5CC+H=C6H6+C2H5 5.8E13 0.0 8.1E3 !<estimated(t)>!
 C6H5CC+OH=C6H5OH+C2H5 1.3E13 0.0 10.6E3 !MF as toluene
 <BAULCH94>as benzene
 C6H5CC+CH3=C7H8+C2H5 1.2E12 0.0 1.24E4 ! MF as benzene-
 kcal <Robaugh, J. Phys. Chem.90(1986)4159 - 4163>
 C6H5CC+O=C6H5CJC+OH 4.2E11 0.0 -2.0
 C6H5CC+OH=C6H5CJC+H2O 3.5E9 1.0 -1.13E3
 C6H5CC+HO2=C6H5CJC+H2O2 2.7E11 0.0 12.0E3
 C6H5CC+O=C6H5CCJ+OH 5.1E8 1.5 5.05E3
 C6H5CC+OH=C6H5CCJ+H2O 3.6E6 2.0 4.82E2
 C6H5CC+HO2=C6H5CCJ+H2O2 4.2E4 2.69 1.85E4
 C6H5CCJ=C2H4+C6H5 2.0E13 0.0 35.5E3
 C6H5CJC+O2=HO2+C6H5C2H3 6.90E11 0.0 15.2E3
 C6H5CCJ+O2=HO2+C6H5C2H3 2.60E11 0.0 2.5E3
 C6H5CJC+HO2=C6H5CPC 3.60E12 0.0 0.0 !MF
 KINGAS
 C6H5CPC=OH+C6H5C(OJ)C 5.00E15 0.0 42500
 !MF
 C6H5C(OJ)C=CH3+C6H5CHO 2.69E13 0.0 12117 !MF as
 but-3-en-1-oxyl <Rauk, Can.J.Chem 81(2003)431-442>

! Styrene submechanism - Herbinet et al. (2013)
 C6H5C2H3+OH=C7H7+CH2O 1.4E12 0.0 -0.9E3 !<as
 butadiene/2!
 C6H5C2H3+OH=C6H5CHO+CH3 1.4E12 0.0 -0.9E3 !MF idem
 réaction précédente as C3H6Y <TSAnG91>
 C6H5C2H3+H=C6H5C2H2+H2 3.3E5 2.53 9.2E3 !MF<as
 butadiene/2>!
 C6H5C2H3+OH=C6H5C2H2+H2O 1.5E6 2.0 0.4E3 !<as
 butadiene/2>!
 C6H5C2H3+CH3=C6H5C2H2+CH4 3.5E13 0.0 15.5E3 !<as
 butadiene/2>
 C6H5C2H2+O2=C6H5CO+CH2O 4.5E16 -1.39 1.0E3
 !<asMebel C2H3+O2>! **

! C7H10 + R
 CH3+CCcyCC*CC*C=CH4+CCcyCJC*CC*C 1.50E+03 2.800 2600
 CH3+CCcyC*CC*CC=CH4+CCcyCJC*CC*C 9.40E+02 2.880 4000
 CH3+CCcyC*CCC*C=CH4+CCcyCJC*CC*C 1.60E+03 2.880 4300
 H+CCcyCC*CC*C=H2+CCcyCJC*CC*C 1.30E+08 1.730 2500
 H+CCcyC*CC*CC=H2+CCcyCJC*CC*C 5.70E+07 1.890 3000
 H+CCcyC*CCC*C=H2+CCcyCJC*CC*C 6.50E+07 1.870 2900
 C3H5-A+CCcyCC*CC*C=C3H6+CCcyCJC*CC*C 3.01E+02 2.970 9160
 C3H5-A+CCcyC*CC*CC=C3H6+CCcyCJC*CC*C 1.91E+02 3.140 11500
 C3H5-A+CCcyC*CCC*C=C3H6+CCcyCJC*CC*C 1.91E+02 3.140 11500

H+Ccy(C*CCCC*C)=H2+Ccy(C*CCCJC*C) 6.60E+08 1.700 2500
 H+Ccy(C*CCCC*C)=H2+Ccy(C*CCJCC*C) 6.60E+08 1.700 2500
 H+Ccy(CC*CC*CC)=H2+Ccy(CCJC*CC*C) 6.60E+08 1.700 2500
 H+Ccy(CC*CC*CC)=H2+Ccy(CJCC*CC*C) 6.60E+08 1.700 2500
 H+Ccy(C*CC*CCC)=H2+Ccy(C*CCCJC*C) 6.60E+08 1.700 2500
 H+Ccy(C*CC*CCC)=H2+Ccy(CJCC*CC*C) 6.60E+08 1.700 2500

H+Ccy (C*CCC*CC)=H2+Ccy (C*CCCJC*C)	5.20E+08	1.710	1900	
H+Ccy (C*CCC*CC)=H2+Ccy (CJCC*CC*C)	5.20E+08	1.710	1900	
H+Ccy (CC*CCC*C)=H2+Ccy (C*CCJCC*C)	5.20E+08	1.710	1900	
H+Ccy (CC*CCC*C)=H2+Ccy (CCJC*CC*C)	5.20E+08	1.710	1900	
CH3+Ccy (CC*CCC*C)=CH4+Ccy (C*CCJCC*C)		2.80E+03	2.890	3500
CH3+Ccy (CC*CCC*C)=CH4+Ccy (CCJC*CC*C)		2.80E+03	2.890	3500
CH3+Ccy (C*CC*CCC)=CH4+Ccy (C*CCCJC*C)		2.90E+03	2.890	3400
CH3+Ccy (C*CC*CCC)=CH4+Ccy (CJCC*CC*C)		2.90E+03	2.890	3400
CH3+Ccy (C*CCC*CC)=CH4+Ccy (C*CCCJC*C)		2.80E+03	2.890	3500
CH3+Ccy (C*CCC*CC)=CH4+Ccy (CJCC*CC*C)		2.80E+03	2.890	3500
CH3+Ccy (C*CCCC*C)=CH4+Ccy (C*CCCJC*C)		2.90E+03	2.890	3400
CH3+Ccy (C*CCCC*C)=CH4+Ccy (C*CCJCC*C)		2.90E+03	2.890	3400
CH3+Ccy (CC*CC*CC)=CH4+Ccy (CCJC*CC*C)		2.90E+03	2.890	3400
CH3+Ccy (CC*CC*CC)=CH4+Ccy (CJCC*CC*C)		2.90E+03	2.890	3400
C3H5-A+Ccy (CC*CCC*C)=C3H6+Ccy (C*CCJCC*C)		3.89E+02	3.120	
9480				
C3H5-A+Ccy (CC*CCC*C)=C3H6+Ccy (CCJC*CC*C)		3.89E+02	3.120	
9480				
C3H5-A+Ccy (C*CCCC*C)=C3H6+Ccy (C*CCCJC*C)		1.88E+02	3.180	
9860				
C3H5-A+Ccy (C*CCCC*C)=C3H6+Ccy (C*CCJCC*C)		1.88E+02	3.180	
9860				
C3H5-A+Ccy (CC*CC*CC)=C3H6+Ccy (CCJC*CC*C)		1.88E+02	3.180	
9860				
C3H5-A+Ccy (CC*CC*CC)=C3H6+Ccy (CJCC*CC*C)		1.88E+02	3.180	
9860				
C3H5-A+Ccy (C*CCC*CC)=C3H6+Ccy (C*CCCJC*C)		3.89E+02	3.120	
9480				
C3H5-A+Ccy (C*CCC*CC)=C3H6+Ccy (CJCC*CC*C)		3.89E+02	3.120	
9480				
C3H5-A+Ccy (C*CC*CCC)=C3H6+Ccy (C*CCCJC*C)		1.88E+02	3.180	
9860				
C3H5-A+Ccy (C*CC*CCC)=C3H6+Ccy (CJCC*CC*C)		1.88E+02	3.180	
9860				
! C8H9 - Vandeputte et al.				
C6H6+C2H3=C*CcyCC*CC*CCJ		6.120e+04	2.410	0.130
! C8H10 + R				
CH3+C*CCcy (C*CC*CC)=CH4+C*CCcyCJC*CC*C		9.40E+02	2.880	4000
CH3+C*CCcy (C*CCC*C)=CH4+C*CCcyCJC*CC*C		1.60E+03	2.880	4300
CH3+C*CCcyCC*CC*C=CH4+C*CCcyCJC*CC*C		1.50E+03	2.800	2600
!C3H5-A+C*CCcy (C*CC*CC)=C3H6+C*CCcyCJC*CC*C		1.91E+02	3.140	11500
!C3H5-A+C*CCcy (C*CCC*C)=C3H6+C*CCcyCJC*CC*C		1.91E+02	3.140	11500
!C3H5-A+C*CCcyCC*CC*C=C3H6+C*CCcyCJC*CC*C		3.01E+02	2.970	9160
C3H5-A+C*CCcy (C*CC*CC)=C3H6+C*CCcyCJC*CC*C		3.85E13		0.000
24179.2				
C3H5-A+C*CCcy (C*CCC*C)=C3H6+C*CCcyCJC*CC*C		3.85E13		0.000
24179.2				
C3H5-A+C*CCcyCC*CC*C=C3H6+C*CCcyCJC*CC*C		8.68E12		0.000
20912.5				
! C10H9 mechanism - Vandeputte et al.				
CPD*CPD+H=CPDcyCJC*CC*C		1.63E+09	1.61	100
CPDcyCJC*CC*C=CPD*cyCC*CCJC		2.46E+08	1.46	16700
CPD*cyCC*CCJC=CPD*cyCC*CCCJ		5.46E+06	2.01	27500
CPDcyCJC*CC*C=tricyclicC10H9		8.89E+11	0.12	9600

tricyclicC10H9=Spiro45_C10H9	7.73E+11	0.31	22900
Spiro45_C10H9=C6H5C*CC*CJ	1.30E+12	0.45	25600
Spiro45_C10H9=tricyclicC10H9f	4.14E+11	0.34	11900
tricyclicC10H9f=C10H9	8.79E+11	0.33	10500
C10H9=C10H8+H	1.34E+08	1.55	15300
C6H5C*CC*CJ=C10H9	3.42E+11	0.22	4800

! C10H10

H+CPDcyCJC*CC*C=C10H10	1.00E+14	0.000	0.000
H+CPD*cyCC*CCJC=C10H10_1	1.00E+14	0.000	0.000
H+CPD*cyCC*CCJC=C10H10_2	1.00E+14	0.000	0.000
H+CPDcyCJC*CC*C=C10H10_2	1.00E+14	0.000	0.000
H+CPD*cyCC*CCCJ=C10H10_3	1.00E+14	0.000	0.000
H+CPDcyCJC*CC*C=C10H10_3	1.00E+14	0.000	0.000
H+CPD*cyCC*CCCJ=C10H10_4	1.00E+14	0.000	0.000
H+CPD*cyCC*CCCJ=C10H10_5	1.00E+14	0.000	0.000
H+CPD*cyCC*CCJC=C10H10_5	1.00E+14	0.000	0.000

! C10H10 + R

C3H5-A+C10H10=C3H6+CPDcyCJC*CC*C	6.02E+02	2.970	9160
C3H5-A+C10H10_1=C3H6+CPD*cyCC*CCJC	3.82E+02	3.140	11500
C3H5-A+C10H10_2=C3H6+CPD*cyCC*CCJC	1.91E+02	3.140	11500
C3H5-A+C10H10_2=C3H6+CPDcyCJC*CC*C	3.01E+02	2.970	9160
C3H5-A+C10H10_3=C3H6+CPD*cyCC*CCCJ	1.91E+02	3.140	11500
C3H5-A+C10H10_3=C3H6+CPDcyCJC*CC*C	3.01E+02	2.970	9160
C3H5-A+C10H10_4=C3H6+CPD*cyCC*CCCJ	1.91E+02	3.140	11500
C3H5-A+C10H10_5=C3H6+CPD*cyCC*CCCJ	1.91E+02	3.140	11500
C3H5-A+C10H10_5=C3H6+CPD*cyCC*CCJC	1.91E+02	3.140	11500
CH3+C10H10=CH4+CPDcyCJC*CC*C	3.00E+03	2.800	2600
CH3+C10H10_1=CH4+CPD*cyCC*CCJC	1.88E+03	2.880	4000
CH3+C10H10_2=CH4+CPD*cyCC*CCJC	9.40E+02	2.880	4000
CH3+C10H10_2=CH4+CPDcyCJC*CC*C	1.50E+03	2.800	2600
CH3+C10H10_3=CH4+CPD*cyCC*CCCJ	9.40E+02	2.880	4000
CH3+C10H10_3=CH4+CPDcyCJC*CC*C	1.50E+03	2.800	2600
CH3+C10H10_4=CH4+CPD*cyCC*CCCJ	9.40E+02	2.880	4000
CH3+C10H10_5=CH4+CPD*cyCC*CCCJ	9.40E+02	2.880	4000
CH3+C10H10_5=CH4+CPD*cyCC*CCJC	9.40E+02	2.880	4000
H+C10H10=H2+CPDcyCJC*CC*C	2.60E+08	1.730	2500
H+C10H10_1=H2+CPD*cyCC*CCJC	1.14E+08	1.890	3000
H+C10H10_2=H2+CPD*cyCC*CCJC	5.70E+07	1.890	3000
H+C10H10_2=H2+CPDcyCJC*CC*C	1.30E+08	1.730	2500
H+C10H10_3=H2+CPD*cyCC*CCCJ	5.70E+07	1.890	3000
H+C10H10_3=H2+CPDcyCJC*CC*C	1.30E+08	1.730	2500
H+C10H10_4=H2+CPD*cyCC*CCCJ	5.70E+07	1.890	3000
H+C10H10_5=H2+CPD*cyCC*CCCJ	5.70E+07	1.890	3000
H+C10H10_5=H2+CPD*cyCC*CCJC	5.70E+07	1.890	3000

! C10H11 mechanism - Vandeputte et al.

C5H5+C5H6=CPDcy(CCJC*CC)	5.65E+01	2.74	3300
CPDcy(CCJC*CC)=CPD1cy(CCJC*CC)	1.12E+08	1.64	22700
CPDcy(CCJC*CC)=CPDC*CC*CCJ	1.58E+11	0.80	41800
CPDC*CC*CCJ=bicyclicC10H11	5.51E+11	0.28	12900
bicyclicC10H11=C4H5cyCCJC*CC*C	7.75E+11	0.44	18700
C4H5cyCCJC*CC*C=C4H5-N+C6H6	7.14E+12	0.52	22900
CPDC*CC*CCJ=CPD1C*CC*CCJ	1.28E+08	1.55	18400
CPD1cy(CCJC*CC)=CPD1C*CC*CCJ	1.71E+10	0.90	31600

CPD1C*CC*CCJ=CPDylC*CC*CC	2.59E+08	1.01	26400
CPDylC*CC*CC=MIndeneJ	7.90E+10	0.29	21100
MIndeneJ=Indene3AH+CH3	3.02E+11	1.22	46300
MIndeneJ=MIndeneJ2	6.07E+06	2.00	26100
MIndeneJ2=C9H8+CH3	1.71E+11	0.86	22700

!*****
!*** Propene oxidation mechanism by Burke et al. ***
!*****

!REF:2 PARAMETER FIT TO HONG ET AL.PROC. OF THE COMB. INST. 33 (2011)
309-316
H+O2<=>O+OH 1.040E+014 0.000
15286.0

!REF:SUTHERLAND ET AL., 21ST SYMPOSIUM, P. 929 (1986)
O+H2<=>H+OH 5.080E+004 2.670
6292.0

!REF:LAM ET AL. SUBMITTED IJCK
OH+H2<=>H+H2O 4.380E+013 0.000
6990.0

!REF:SUTHERLAND ET AL., 23RD SYMPOSIUM, P. 51 (1990)
O+H2O<=>OH+OH 2.970E+006 2.020
13400.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
H2+M<=>H+H+M 4.577E+019 -1.400
104400.0
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 6.165E+015 -0.500
0.0
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 4.714E+018 -1.000
0.0
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 3.500E+022 -2.000
0.0

!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) 4.650E+012 0.440
0.0
LOW/ 1.737E+019 -1.230
0.0/
TROE/ 6.700E-001 1.000E-030 1.000E+030 1.000E+030/

H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/
C2H6/ 3.00/
H+O2 (+AR) <=>HO2 (+AR) 4.650E+012 0.440
0.0

!REF: BATES ET AL. PCCP 3 (2001) 2337-2342
LOW/ 6.810E+018 -1.200
0.0/
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:KEYSER, J. PHYS. CHEM. 92:1193 (1988) REDUCED BY 15%
HO2+OH<=>H2O+O2 2.456E+013 0.000
-497.0

!REF:HIPPLER ET AL. J.CHEM.PHYS 93 1755-1760 (1990)
HO2+HO2<=>H2O2+O2 1.300E+011 0.000
-1630.0
DUP

!REF:REDUCED BY 13%
HO2+HO2<=>H2O2+O2 3.658E+014 0.000
12000.0
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 0.0	3.020E+013	0.000
HCO+O<=>CO2+H 0.0	3.000E+013	0.000
!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	1.500E+013	0.000
H2/ 1.00/ H2O/ 6.50/ O2/ 0.40/ N2/ 0.40/ AR/ 0.35/ OH*+H2O<=>OH+H2O -860.0	5.930E+012	0.500
OH*+H2<=>OH+H2 -444.0	2.950E+012	0.500
OH*+N2<=>OH+N2 -1242.0	1.080E+011	0.500

OH*+OH<=>OH+OH	6.010E+012	0.500
-764.0		
OH*+H<=>OH+H	1.310E+012	0.500
-167.0		
OH*+AR<=>OH+AR	1.690E+012	0.000
4135.0		
OH*<=>OH	1.450E+006	0.000
0.0		
OH*+O2<=>OH+O2	2.100E+012	0.500
-478.0		
OH*+CO2<=>OH+CO2	2.750E+012	0.500
-968.0		
OH*+CO<=>OH+CO	3.230E+012	0.500
-787.0		
OH*+CH4<=>OH+CH4	3.360E+012	0.500
-635.0		
CH+O2<=>CO+OH*	4.040E+013	0.000
0.0		
C2H+O<=>CO+CH*	6.200E+012	0.000
0.0		
C+H+M<=>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<=>CO2+CH*	2.170E+010	0.000
0.0		

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

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

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

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

HOCHO+H=>H2+CO2+H 4868.0	4.240E+006	2.100
!REF:MARINOV ESTIMATE		
HOCHO+H=>H2+CO+OH 2988.0	6.030E+013	-0.350
HOCHO+CH3=>CH4+CO+OH 2200.0	3.900E-007	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	6.800E+013	0.000
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/	1.867E+025	-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)	5.400E+011	0.454
3600.0		
LOW/	1.270E+032	-4.820
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/		
!REF:GROTHER, H. H. ET AL., J. PHYS. CHEM. 92: 4028 (1988).		
CH2OH+O2<=>CH2O+HO2	1.510E+015	-1.000
0.0		
DUP		
CH2OH+O2<=>CH2O+HO2	2.410E+014	0.000
5017.0		
DUP		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH2OH+H<=>CH2O+H2	6.000E+012	0.000
0.0		
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+HO2<=>CH2O+H2O2	1.200E+013	0.000
0.0		
!REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998)		
CH2OH+HCO<=>CH2O+CH2O	1.800E+014	0.000
0.0		
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+CH3O<=>CH2O+CH3OH	2.400E+013	0.000
0.0		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+HCO<=>CH2OH+CH2O	9.630E+003	2.900
13110.0		
OH+CH2OH<=>H2O+CH2O	2.400E+013	0.000
0.0		
O+CH2OH<=>OH+CH2O	4.200E+013	0.000
0.0		
CH2OH+CH2OH<=>CH2O+CH3OH	3.000E+012	0.000
0.0		
!REF:CURRAN ESTIMATE		
CH2OH+HO2<=>HOCH2O+OH	1.000E+013	0.000
0.0		
CH2O+HO2<=>OCH2O2H	1.500E+011	0.000
11900.0		
OCH2O2H<=>HOCH2O2	3.000E+011	0.000
8600.0		
HOCH2O2+HO2<=>HOCH2O2H+O2	3.500E+010	0.000
-3275.0		
HOCH2O+OH<=>HOCH2O2H	1.000E+013	0.000
0.0		
!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)	2.084E+018	-0.615
92540.6		

LOW/ 97992.2/ TROE/ -4.748E-001 3.558E+004 1.116E+003 9.023E+003/ CH3OH (+M) <=> CH2 (S) + H2O (+M) 91712.0	1.500E+043	-6.995
LOW/ 99417.1/ TROE/ 2.545E+000 3.290E+003 4.732E+004 4.711E+004/ CH3OH (+M) <=> CH2OH+H (+M) 84467.4	1.430E+047	-8.227
LOW/ 105230.3/ TROE/ -7.391E+001 3.705E+004 4.150E+004 5.220E+003/	3.390E+042	-7.244
!REF:J. CHEM. PHYS. 134, 094302 (2011)		
CH3OH+H<=>CH2OH+H2 5440.0	3.070E+005	2.550
CH3OH+H<=>CH3O+H2 10300.0	1.990E+005	2.560
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+O<=>CH2OH+OH 3080.0	3.880E+005	2.500
!REF:XU ET AL. PROC 31 2007 159-166		
CH3OH+OH<=>CH2OH+H2O -806.7	3.080E+004	2.650
CH3OH+OH<=>CH3O+H2O -763.0	1.500E+002	3.030
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
CH3OH+O2<=>CH2OH+HO2 44900.0	2.050E+013	0.000
!REF:CURRAN ESTIMATE		
CH3OH+HO2<=>CH2OH+H2O2 10530.0	1.080E+004	2.550
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+CH3<=>CH2OH+CH4 7172.0	3.190E+001	3.170
CH3O+CH3OH<=>CH2OH+CH3OH 4074.0	3.000E+011	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3O+CH3O<=>CH3OH+CH2O 0.0	6.030E+013	0.000
!REF:GRI		
CH3+H (+M) <=> CH4 (+M) 383.0	1.270E+016	-0.630
LOW/ 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/	2.477E+033	-4.760

!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 1.810E+012 0.000
13710.0

!REF:KEIFFER, M. ET AL., J. CHEM. SOC. FARADAY TRANS. 2: 84, 505 (1988)

CH3O2+CH3<=>CH3O+CH3O 5.080E+012 0.000
-1411.0

!REF: LIGHTFOOT, P.D. ETAL., ATMOS. ENVIRON. PART A: 26, 1805-1961 (1992)

CH3O2+HO2<=>CH3O2H+O2 2.470E+011 0.000
-1570.0

!REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220.

CH3O2+CH3O2=>CH2O+CH3OH+O2 3.110E+014 -1.610
-1051.0

CH3O2+CH3O2=>O2+CH3O+CH3O 1.400E+016 -1.610
1860.0

CH3O2+H<=>CH3O+OH 9.600E+013 0.000
0.0

CH3O2+O<=>CH3O+O2 3.600E+013 0.000
0.0

CH3O2+OH<=>CH3OH+O2 6.000E+013 0.000
0.0

CH3O2H<=>CH3O+OH 6.310E+014 0.000
42300.0

!REF:GRI

CH2(S)+N2<=>CH2+N2 1.500E+013 0.000
600.0

CH2(S)+AR<=>CH2+AR 9.000E+012 0.000
600.0

CH2(S)+H<=>CH+H2 3.000E+013 0.000
0.0

CH2(S)+O<=>CO+H2 1.500E+013 0.000
0.0

CH2(S)+O<=>HCO+H 1.500E+013 0.000
0.0

CH2(S)+OH<=>CH2O+H 3.000E+013 0.000
0.0

CH2(S)+H2<=>CH3+H 7.000E+013 0.000
0.0

CH2(S)+O2=>H+OH+CO 2.800E+013 0.000
0.0

CH2(S)+O2<=>CO+H2O 1.200E+013 0.000
0.0

CH2(S)+H2O<=>CH2+H2O 3.000E+013 0.000
0.0

CH2(S)+CO<=>CH2+CO 9.000E+012 0.000
0.0

CH2(S)+CO2<=>CH2+CO2 7.000E+012 0.000
0.0

CH2 (S) + CO2 <=> CH2O + CO 1.400E+013 0.000
0.0

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

CH2+H (+M) <=> CH3 (+M) 2.500E+016 -0.800
0.0

LOW/ 3.200E+027 -3.140
1230.0/

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

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!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/

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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/	1.030E+059	-11.300
95912.5/		
TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/		
CH3CHO (+M) <=>CH4+CO (+M)	2.720E+021	-1.740
86355.0		
LOW/	1.144E+058	-11.300
95912.5/		
TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/		
!REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010		
CH3CHO+H<=>CH3CO+H2	1.310E+005	2.580
1220.0		
CH3CHO+H<=>CH2CHO+H2	2.720E+003	3.100
5210.0		
!REF:CURRAN, FIT TO NIST DATABASE		
CH3CHO+O<=>CH3CO+OH	5.940E+012	0.000
1868.0		
!REF:JUAN LI'S PHD THESIS		
CH3CHO+OH<=>CH3CO+H2O	3.370E+012	0.000
-619.0		
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+O2<=>CH3CO+HO2	3.010E+013	0.000
39150.0		
!REF: GUPTA ET AL., PROC COMBUST INST 31 (2007) 167-174		
CH3CHO+CH3<=>CH3CO+CH4	7.080E-004	4.580
1966.0		
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+HO2<=>CH3CO+H2O2	3.010E+012	0.000
11920.0		
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3O2+CH3CHO<=>CH3O2H+CH3CO	3.010E+012	0.000
11920.0		
CH3CHO+CH3CO3<=>CH3CO+CH3CO3H	3.010E+012	0.000
11920.0		
!REF:TAYLOR ET AL. 1996		
CH3CHO+OH<=>CH3+HOCHO	3.000E+015	-1.076
0.0		
CH3CHO+OH<=>CH2CHO+H2O	1.720E+005	2.400
815.0		
!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781		
CH3CO (+M) <=>CH3+CO (+M)	1.070E+012	0.630
16900.0		

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 0.0	2.000E+013	0.000
CH3CO+CH3<=>CH2CO+CH4 0.0	5.000E+013	0.000
!REF:		
CH3CO+O2<=>CH3CO3 -1100.0	1.200E+011	0.000
CH3CO3+HO2<=>CH3CO3H+O2 -3275.0	1.750E+010	0.000
H2O2+CH3CO3<=>HO2+CH3CO3H 9936.0	2.410E+012	0.000
CH4+CH3CO3<=>CH3+CH3CO3H 18480.0	1.810E+011	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
!REF:ANALOGY TO CH3O2+CH2O		
CH2O+CH3CO3<=>HCO+CH3CO3H 11660.0	1.990E+012	0.000
!REF: ANALOGY TO C2H6+HO2		
C2H6+CH3CO3<=>C2H5+CH3CO3H 20460.0	1.700E+013	0.000
!REF:SAHETCHIAN ET AL. 1992		
CH3CO3H<=>CH3CO2+OH 40150.0	5.010E+014	0.000
!REF:ANALOGY TO CH3CO<=>CH3+CO		
CH3CO2+M<=>CH3+CO2+M 10500.0	4.400E+015	0.000
!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781		
CH2CHO (+M) <=> CH2CO+H (+M) 45600.0	1.430E+015	-0.150
!REF:LPL TIMES 2		
LOW/ 43423.9/ TROE/ 9.850E-001 3.930E+002 9.800E+009 5.000E+009/	6.000E+029	-3.800
!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781		
CH2CHO (+M) <=> CH3+CO (+M) 40300.0	2.930E+012	0.290
LOW/ 41300.0/ TROE/ 7.130E-017 1.150E+003 4.990E+009 1.790E+009/	9.520E+033	-5.070
!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) \rightleftharpoons 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 \rightleftharpoons HCCO+H2	1.401E+015	-0.171
8783.2		
CH2CO+H \rightleftharpoons CH3+CO	7.704E+013	-0.171
4183.2		

!REF:CURRAN ESTIMATE

CH2CO+O \rightleftharpoons CH2+CO2	1.750E+012	0.000
1350.0		

!REF:

CH2CO+O \rightleftharpoons HCCO+OH	1.000E+013	0.000
8000.0		
CH2CO+OH \rightleftharpoons HCCO+H2O	1.000E+013	0.000
2000.0		

!REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491.

CH2CO+OH \rightleftharpoons CH2OH+CO	2.000E+012	0.000
-1010.0		

!REF:WKM CALCULATION, CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT

CH2CO+CH3 \rightleftharpoons C2H5+CO	4.769E+004	2.312
9468.0		
CH2(S)+CH2CO \rightleftharpoons C2H4+CO	1.600E+014	0.000
0.0		
HCCO+OH \rightleftharpoons H2+CO+CO	1.000E+014	0.000
0.0		
HCCO+O \rightleftharpoons H+CO+CO	8.000E+013	0.000
0.0		

!REF:GRI

HCCO+H \rightleftharpoons CH2(S)+CO	1.000E+014	0.000
0.0		

!REF:KLIPPENSTEIN 2002

HCCO+O2 \rightleftharpoons OH+CO+CO	1.910E+011	-0.020
1020.0		
HCCO+O2 \rightleftharpoons CO2+CO+H	4.780E+012	-0.142
1150.0		

!REF:FULLE, D.; HIPPLER, H.; STRIEBEL, F.

!REF:J. CHEM. PHYS. 108: 6709-6716 1998

CH+CO+M \rightleftharpoons HCCO+M	7.570E+022	-1.900
0.0		

!REF:REG 2.11

CH+CH2O<=>H+CH2CO	9.460E+013	0.000
-515.0		
CH+HCCO<=>CO+C2H2	5.000E+013	0.000
0.0		
!REF:GRI 3.0		
C2H3+H (+M) <=>C2H4 (+M)	6.080E+012	0.270
280.0		
LOW/	1.400E+030	-3.860
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/		
!REF:GRI		
C2H4 (+M) <=>H2+H2CC (+M)	8.000E+012	0.440
88770.0		
LOW/	7.000E+050	-9.310
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/		
!REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996)		
C2H4+H<=>C2H3+H2	5.070E+007	1.930
12950.0		
!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 1.130E+013 0.000
30430.0

!REF:PITZ ESTIMATE
C2H4+CH3O2<=>C2H4O1-2+CH3O 2.820E+012 0.000
17110.0
C2H4+C2H5O2<=>C2H4O1-2+C2H5O 2.820E+012 0.000
17110.0

!REF:BAULCH AND COBOS REDUCED BY A FACTOR OF 4
C2H4+HO2<=>C2H4O1-2+OH 5.575E+011 0.000
17190.0

!REF:BUTLER, FLEMING, GOSS, LIN, ACS SYMP. SER. 134 (1980).
CH+CH4<=>C2H4+H 6.000E+013 0.000
0.0

!REF:MARINOV ESTIMATE.
CH2(S)+CH3<=>C2H4+H 2.000E+013 0.000
0.0

!REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202
C2H2+H(+M)<=>C2H3(+M) 1.710E+010 1.266
2709.0
LOW/ 6.346E+031 -4.664
3780.0/
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

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!REF:ADOPTING KLIPPENSTEIN'S PRODUCTS FOR ONE OF THE CHANNELS,

!REF:TO COMBAT OVER-PRODUCTION OF C2H2 IN ETHYLENE JSR
!C2H3+O2<=>CH2O+HCO          2.380E+027   -4.859
4912.3
!C2H3+O2<=>CH2CHO+O          5.340E+012   -0.013
3322.7
!C2H3+O2=>H+CO+CH2O          3.380E+014   -0.885
2176.7

!REF:
CH3+C2H3<=>CH4+C2H2          3.920E+011    0.000
0.0

!REF:86TSA/ HAM
C2H3+H<=>C2H2+H2            9.000E+013    0.000
0.0

!REF:USC ESTIMATE
C2H3+H<=>H2CC+H2            6.000E+013    0.000
0.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
C2H3+OH<=>C2H2+H2O          3.011E+013    0.000
0.0
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

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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	12420.0/	
PLOG/	0.0250	7.467E+005	2.160	12550.0/	
PLOG/	0.1000	1.776E+006	2.040	12670.0/	
PLOG/	1.0000	2.415E+006	2.000	12710.0/	
PLOG/	10.0000	3.210E+006	1.970	12810.0/	
PLOG/	100.0000	7.347E+006	1.890	13600.0/	
C2H2+OH<=>CH2CO+H				1.578E+003	2.560
-844.5					
PLOG/	0.0100	1.578E+003	2.560	-844.5/	
PLOG/	0.0250	1.518E+004	2.280	-292.1/	
PLOG/	0.1000	3.017E+005	1.920	598.1/	
PLOG/	1.0000	7.528E+006	1.550	2106.0/	
PLOG/	10.0000	5.101E+006	1.650	3400.0/	
PLOG/	100.0000	1.457E+004	2.450	4477.0/	
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 7475.1		2.450E-005		5.260
C2H5OH+HO2<=>PC2H4OH+H2O2 15333.0		3.986E-002		4.300
C2H5OH+HO2<=>C2H5O+H2O2 10533.1		6.470E-007		5.300
!REF:ANAOLGY WITH C2H5OH+HO2				
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H 7475.1		1.225E-005		5.260
C2H5OH+CH3O2<=>PC2H4OH+CH3O2H 15333.0		1.995E-002		4.300
C2H5OH+CH3O2<=>C2H5O+CH3O2H 10533.1		3.236E-007		5.300
!REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703				
C2H5OH+O<=>PC2H4OH+OH 4658.0		9.690E+002		3.230
C2H5OH+O<=>SC2H4OH+OH 876.0		1.450E+005		2.470
C2H5OH+O<=>C2H5O+OH 1727.0		1.460E-003		4.730
!REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004				
C2H5OH+CH3<=>PC2H4OH+CH4 12290.0		3.300E+002		3.300
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
!REF:ESTIMATE				
C2H5OH+C2H5<=>SC2H4OH+C2H6 10400.0		5.000E+010		0.000
!REF:CURRAN, FIT TO NIST DATABASE				
!REF:WKM CALCULATION.				
SC2H4OH<=>CH3CHO+H 45049.0		5.690E+052		-13.380
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
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				5.480E+045	-11.630
44328.0					
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				2.650E+036	-8.860
51019.0					
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:ESTIMATE CH3COCH3+OH<=>CH3COCH2+H2O 445.0	1.250E+005	2.483
!REF:CURRAN ESTIMATE CH3COCH3+H<=>CH3COCH2+H2 5160.0	9.800E+005	2.430
!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98 CH3COCH3+O<=>CH3COCH2+OH 4890.0	5.130E+011	0.211
!REF: CH3COCH3+CH3<=>CH3COCH2+CH4 9784.0	3.960E+011	0.000
!REF:ESTIMATE CH3COCH3+CH3O<=>CH3COCH2+CH3OH 6460.0	4.340E+011	0.000
!REF:A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN CH3COCH3+O2<=>CH3COCH2+HO2 48500.0	6.030E+013	0.000
!REF:ANALOGY TO ETHANE CH3COCH3+HO2<=>CH3COCH2+H2O2 20460.0 CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H 20460.0	1.700E+013 1.700E+013	0.000 0.000
!REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 CH2CO+CH3<=>CH3COCH2 6130.0 CH3COCH2+HO2<=>CH3COCH2O+OH 0.0 CH3COCH2+CH3O2<=>CH3COCH2O+CH3O 0.0 CH3COCH2+H<=>CH3COCH3 0.0 CH3COCH2O<=>CH3CO+CH2O 5108.0	1.760E+004 2.410E+013 1.205E+013 1.000E+013 5.000E+010	2.480 0.000 0.000 0.000 0.000
!REF: CH3COCH2+O2<=>CH3COCH2O2 -1100.0	1.200E+011	0.000
!REF:WESTBROOK ESTIMATE CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21 5000.0 CH2O+CH3COCH2O2<=>HCO+C3KET21 9000.0 HO2+CH3COCH2O2<=>C3KET21+O2 0.0	1.000E+011 1.288E+011 1.000E+012	0.000 0.000 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 C2H5CHO+C2H5O<=>C2H5CO+C2H5OH 3300.0	1.000E+012 6.026E+011	0.000 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:COOK ET AL. J. PHYS. CHEM A 2009, 113, 9974-9980 CH3OCH3 (+M) <=> CH3+CH3O (+M) 83890.0 LOW/ 42790.0/ TROE/ 4.540E-001 1.000E-030 2.510E+003/	4.380E+021 7.520E+015	-1.570 0.000
!REF:ARIF M, ET AL., J. PHYS. CHEM. A, 101, 13, 2436-2441 (1997). CH3OCH3+OH<=>CH3OCH2+H2O -651.7	6.324E+006	2.000
!REF:CURRAN, FIT TO NIST DATABASE CH3OCH3+H<=>CH3OCH2+H2 3384.0	7.721E+006	2.090
!REF:CURRAN 08 NIST FIT CH3OCH3+O<=>CH3OCH2+OH 2250.0	7.750E+008	1.360
!REF:BASED ON J. AGUILERA-IPARRAGUIRRE ET AL !REF:J PHYS CHEM A (2008) 112(30): 7047-7054. !REF:THE A-FACTOR FOR ABSTRACTION BY HO2 AND CH3O2 WAS MULTIPLIED BY 0.5		

CH3OCH3+HO2<=>CH3OCH2+H2O2 12090.0	8.670E+002	3.010
CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H 13190.0	3.120E+002	3.120
!REF:		
CH3OCH3+CH3<=>CH3OCH2+CH4 5700.0	1.445E-006	5.730
CH3OCH3+O2<=>CH3OCH2+HO2 44910.0	4.100E+013	0.000
!REF:ESTIMATE		
CH3OCH3+CH3O<=>CH3OCH2+CH3OH 4074.0	6.020E+011	0.000
!REF:		
CH3OCH3+CH3OCH2O2<=>CH3OCH2+CH3OCH2O2H 17690.0	5.000E+012	0.000
CH3OCH3+O2CHO<=>CH3OCH2+HO2CHO 13910.0	4.425E+004	2.600
CH3OCH3+OCHO<=>CH3OCH2+HOCHO 17690.0	1.000E+013	0.000
CH3OCH2<=>CH2O+CH3 25500.0	1.600E+013	0.000
!REF:ESTIMATE		
CH3OCH2+CH3O<=>CH3OCH3+CH2O 0.0	2.410E+013	0.000
CH3OCH2+CH2O<=>CH3OCH3+HCO 5862.0	5.490E+003	2.800
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO 8499.0	1.260E+012	0.000
CH3OCH2+O2<=>CH3OCH2O2 0.0	2.000E+012	0.000
!REF:!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
!REF:!1/ 2 CH3O2+CH2O<=>CH3O2H+HCO		
CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO 11660.0	1.000E+012	0.000
!REF:ESTIMATE		
CH3OCH2O2+CH3CHO<=>CH3OCH2O2H+CH3CO 13600.0	2.800E+012	0.000
CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O 0.0	1.547E+023	-4.500
CH3OCH2O+OH<=>CH3OCH2O2H 0.0	2.000E+013	0.000
CH3O+CH2O<=>CH3OCH2O 7960.0	1.000E+011	0.000
CH3OCH2O+O2<=>CH3OCHO+HO2 500.0	5.000E+010	0.000
!REF:		
CH3OCHO+H<=>CH3OCH2O 7838.0	1.000E+013	0.000
!REF:ESTIMATE EA EQUALS DELTAH+RS+EABS		

CH3OCH2O2<=>CH2OCH2O2H 21580.0	6.000E+010	0.000
!REF: ESTIMATE EA<=>DELTAU+EADDN.		
CH2OCH2O2H=>OH+CH2O+CH2O 20760.0	1.500E+013	0.000
!REF:ESTIMATE		
CH2OCH2O2H+O2<=>O2CH2OCH2O2H 0.0	7.000E+011	0.000
O2CH2OCH2O2H<=>HO2CH2OCHO+OH 18580.0	4.000E+010	0.000
HO2CH2OCHO<=>OCH2OCHO+OH 40500.0	2.000E+016	0.000
!REF:WKM RECOMMENDATION 8/ 9/ 2010		
!REF:ESTIMATE		
CH2O+OCHO<=>OCH2OCHO 11900.0	1.250E+011	0.000
OCH2OCHO<=>HOCH2OCO 14000.0	1.000E+011	0.000
HOCH2O+CO<=>HOCH2OCO 4800.0	1.500E+011	0.000
CH2OH+CO2<=>HOCH2OCO 35720.0	1.500E+011	0.000
!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.		
CH2OCHO+H<=>CH3OCHO 0.0	1.000E+014	0.000
CH3OCO+H<=>CH3OCHO 0.0	1.000E+014	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		2.755E+005		2.450
2830.0				
!REF: FIT TO COHEN/ WESTBERG '86				
CH3OCHO+O<=>CH2OCHO+OH		9.800E+005		2.430
4750.0				
!REF:1/ 2 TSANG'S C3H8+H				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+H<=>CH3OCO+H2		6.500E+005		2.400
4471.0				
CH3OCHO+H<=>CH2OCHO+H2		6.650E+005		2.540
6756.0				
!REF:C3H8+CH3<=>IC3H7+CH4				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+CH3<=>CH3OCO+CH4		7.550E-001		3.460
5481.0				
!REF:C3H8+CH3<=>NC3H7+CH4				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+CH3<=>CH2OCHO+CH4		4.520E-001		3.650
7154.0				
!REF:ESTIMATE				
CH3OCHO+CH3O<=>CH3OCO+CH3OH		5.480E+011		0.000
5000.0				
CH3OCHO+CH3O<=>CH2OCHO+CH3OH		2.170E+011		0.000
6458.0				
!REF:ANALOGY WITH HO2				
CH3OCHO+CH3O2<=>CH3OCO+CH3O2H		4.820E+003		2.600
13910.0				
CH3OCHO+CH3O2<=>CH2OCHO+CH3O2H		2.380E+004		2.550
16490.0				
!REF:C3H8+HCO				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+HCO<=>CH3OCO+CH2O		5.400E+006		1.900
17010.0				
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				1.054E+010	0.970
1586.0					

C3H8+OH<=>IC3H7+H2O				4.670E+007	1.610
-35.0					

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

C3H8+HO2<=>IC3H7+H2O2				6.320E+001	3.370
13720.0					

C3H8+HO2<=>NC3H7+H2O2				4.080E+001	3.590
17160.0					

!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) 0.0	2.500E+013	0.000
LOW/ 9769.8/	4.270E+058	-11.940
TROE/ 1.750E-001 1.341E+003 6.000E+004 1.014E+004/		
C3H5-A+H (+M) <=> C3H6 (+M) 0.0	1.000E+014	0.000
LOW/ 5967.8/	6.650E+059	-12.000
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 140000.0	7.710E+069	-16.090
C3H6<=>C3H5-T+H 139300.0	5.620E+071	-16.580

!REF: ANALOGY WITH C2H4

C3H6+O<=>C2H5+HCO 183.0	7.450E+006	1.880
C3H6+O=>CH2CO+CH3+H 183.0	3.050E+006	1.880
C3H6+O=>CH3CHCO+H+H 183.0	3.050E+006	1.880
C3H6+O<=>C3H5-A+OH 5884.0	5.240E+011	0.700
C3H6+O<=>C3H5-S+OH 8959.1	1.200E+011	0.700
C3H6+O<=>C3H5-T+OH 7632.0	6.030E+010	0.700

!REF: TOTAL RATE ZADOR (PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053)/VASU (J. PHYS. CHEM. A 2010, 114, 11529-11537) ALTERED BRANCHING RATIO

C3H6+OH<=>C3H5-A+H2O 1050.8	4.460E+006	2.072
C3H6+OH<=>C3H5-S+H2O 2502.0	1.860E+005	2.369
C3H6+OH<=>C3H5-T+H2O 2235.2	1.800E+006	1.979

!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 2600.0	8.400E+010	0.000
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!REF: C3 NUIG CALCULATION J.M

C3H6+HO2<=>C3H5-S+H2O2 20798.6	9.570E+002	3.059
C3H6+HO2<=>C3H5-T+H2O2 24427.9	1.560E+004	2.820
C3H6+HO2<=>IC3H7O2 5109.0	1.050E-025	3.520
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 11201.0	4.850E-021	2.650
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 23587.0	1.130E+019	-1.680
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/	
PLOG/	100.0000	7.240E+026	-4.210	6825.0/	
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	1.440E+032	-6.010	6053.6/		
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 3.47E+06 1.53 4288/

PLOG/ 0.0100 1.08E+07 1.34 4576/

PLOG/ 0.0130 9.76E+06 1.33 4589/

PLOG/ 0.0250 5.14E+06 1.36 4594/

PLOG/ 0.1000 3.13E+05 1.69 4603/

PLOG/ 0.1315 1.39E+05 1.80 4603/

PLOG/ 1.0000 1.03E+02 2.83 4530/

PLOG/ 10.0000 3.40E-02 3.89 4390/

PLOG/ 100.0000 4.46E-06 5.03 4132/

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/	
DUP					
C3H6+OH<=>C3H6OH2-1				1.420E+036	-15.840
11594.0					
PLOG/	0.0013	7.680E+077	-20.700	32402.0/	
PLOG/	0.0100	9.130E+076	-20.000	33874.0/	
PLOG/	0.0130	3.550E+075	-19.580	32874.0/	
PLOG/	0.0250	1.230E+073	-18.790	31361.0/	
PLOG/	0.1000	3.450E+067	-17.010	27909.0/	
PLOG/	0.1315	2.410E+066	-16.640	27162.0/	
PLOG/	1.0000	6.500E+058	-14.170	23079.0/	
PLOG/	10.0000	2.530E+053	-12.230	22976.0/	
PLOG/	100.0000	4.780E+047	-10.230	23772.0/	

DUP

!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 3.000E+013 0.000
39100.0

!REF: TSANG 1991

SC3H5OH+OH=>C2H3CHO+H+H2O 3.100E+006 2.000
-298.0

SC3H5OH+H=>C2H3CHO+H+H2 1.730E+005 2.500
2492.0

SC3H5OH+O=>C2H3CHO+H+OH 1.750E+012 0.700
5884.0

SC3H5OH+HO2=>C2H3CHO+H+H2O2 9.600E+003 2.600
13900.0

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

!REF: USE HO2 ABSTRACTION RATE CONSTANT

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

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

!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

!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				
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			2.000E+007	1.800
1000.0				
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).				
C3H4-A+O<=>C2H2+CH2O			3.000E-003	4.610
-4243.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
!C3H4-A+CH3<=>C3H3+CH4			1.300E+012	0.000
7700.0				
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).				
!C3H4-A+C3H5-A<=>C3H3+C3H6			2.000E+011	0.000
7700.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H4-A+C2H<=>C2H2+C3H3			1.000E+013	0.000
0.0				
!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589				
C3H4-P+H<=>C3H5-A			1.100E+060	-14.560
28100.0				
PLOG/	0.1000	1.100E+060	-14.560	28100.0/
PLOG/	1.0000	4.910E+060	-14.370	31644.0/
PLOG/	2.0000	3.040E+060	-14.190	32642.0/
PLOG/	5.0000	9.020E+059	-13.890	33953.0/
PLOG/	10.0000	2.200E+059	-13.610	34900.0/
PLOG/	100.0000	1.600E+055	-12.070	37500.0/
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H4-P+C3H3<=>C3H4-A+C3H3			6.140E+006	1.740
10450.0				
!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 -304.0	2.220E+012	0.000
!REF: ANALOGY with Curran 2006 alkyl decomp		
CH2CCH2OH<=>CH2O+C2H3 30460.0	9.240E+010	0.870
CH2CCH2OH<=>C2H3CHO+H 36770.0	1.110E+011	0.480
CH2CCH2OH<=>HCO+C2H4 30460.0	9.240E+010	0.870
!SC3H4OH<=>CH2CO+CH3 30460.0	9.240E+010	0.870
!C3H4-A+H<=>C3H3+H2 5522.0	6.625E+003	3.095
!REF: analogies with c3h6 a and s		
C3H4-P+OH<=>C3H3+H2O 1059.6	4.940E+006	2.027
C3H4-A+OH<=>C3H3+H2O 1807.2	1.482E+005	2.492
!C3H4-P+H<=>C3H3+H2 4821.0	3.572E+004	2.825
!REF: ESTIMATES C3 NUIG S.M.B from Atkinson 1982 and 1984		
C3H4-P+OH<=>PC3H4OH-2 0.0	3.930E+011	0.000
C3H4-P+OH<=>SC3H4OH 0.0	2.360E+012	0.000
!REF: Matheu et al. IJCK, 2003, 35, 95--119		
PC3H4OH-2<=>CH3CHCHO 23238.0	3.560E+010	0.880
!REF: Pelucchi ECM 2013		
!CH3CHCHO<=>C2H3CHO+H 32410.0	4.164E+012	-0.020

!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+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+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					
IC3H7+O2<=>IC3H7O2				7.540E+012	0.000
0.0					
!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 30430.0	1.130E+013	0.000
!REF:ANALOGY TO CH3OH+HO2		
CH3OH+NC3H7O2<=>CH2OH+NC3H7O2H 19360.0	6.300E+012	0.000
CH3OH+IC3H7O2<=>CH2OH+IC3H7O2H 19360.0	6.300E+012	0.000
!REF:HALF OF CH2O+HO2		
C2H3CHO+NC3H7O2<=>C2H3CO+NC3H7O2H 13600.0	2.800E+012	0.000
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:
 $C_3H_6 + HO_2 \rightleftharpoons C_3H_6OOH_1 - 2$ 1.000E+011 0.000
 11000.0
 $C_3H_6OOH_1 - 3 \Rightarrow OH + CH_2O + C_2H_4$ 3.035E+015 -0.790
 27400.0

!REF:BOZZELLI AND PITZ, 1995
 $C_3H_6OOH_2 - 1 \rightleftharpoons C_2H_3OOH + CH_3$ 6.540E+027 -5.140
 38320.0
 $C_3H_6OOH_1 - 2 \Rightarrow C_2H_4 + CH_2O + OH$ 1.310E+033 -7.010
 48120.0

!REF:ESTIMATE
 $C_3H_6OOH_2 - 2 \rightleftharpoons CH_3COCH_3 + OH$ 9.000E+014 0.000
 1500.0
 $C_3H_6OOH_1 - 2 + O_2 \rightleftharpoons C_3H_6OOH_1 - 2O_2$ 5.000E+012 0.000
 0.0
 $C_3H_6OOH_1 - 3 + O_2 \rightleftharpoons C_3H_6OOH_1 - 3O_2$ 4.520E+012 0.000
 0.0
 $C_3H_6OOH_2 - 1 + O_2 \rightleftharpoons C_3H_6OOH_2 - 1O_2$ 4.520E+012 0.000
 0.0

!REF:
 $C_3H_6OOH_1 - 2O_2 \rightleftharpoons C_3KET12 + OH$ 6.000E+011 0.000
 26400.0
 $C_3H_6OOH_1 - 3O_2 \rightleftharpoons C_3KET13 + OH$ 7.500E+010 0.000
 21400.0
 $C_3H_6OOH_2 - 1O_2 \rightleftharpoons C_3KET21 + OH$ 3.000E+011 0.000
 23850.0
 $C_3H_6OOH_2 - 1O_2 \rightleftharpoons C_3H_51 - 2, 3OOH$ 1.125E+011 0.000
 24400.0
 $C_3H_6OOH_1 - 2O_2 \rightleftharpoons C_3H_51 - 2, 3OOH$ 9.000E+011 0.000
 29400.0

!REF: BOZZELLI AND PITZ, 1993.
 $C_3H_51 - 2, 3OOH \rightleftharpoons AC_3H_5OOH + HO_2$ 2.560E+013 -0.490
 17770.0

!REF:
 $C_3H_6OOH_1 - 3O_2 \rightleftharpoons C_3H_52 - 1, 3OOH$ 6.000E+011 0.000
 26850.0

!REF:BOZZELLI AND PITZ, 1993.
 $C_3H_52 - 1, 3OOH \rightleftharpoons AC_3H_5OOH + HO_2$ 1.150E+014 -0.630
 17250.0

!REF:
 $C_3KET12 \Rightarrow CH_3CHO + HCO + OH$ 9.450E+015 0.000
 43000.0
 $C_3KET13 \Rightarrow CH_2O + CH_2CHO + OH$ 1.000E+016 0.000
 43000.0
 $C_3KET21 \Rightarrow CH_2O + CH_3CO + OH$ 1.000E+016 0.000
 43000.0

!REF:ESTIMATE

!REF:

!REF:ACETALDEHYDE ANALOG
C3H5O+O2<=>C2H3CHO+HO2 1.000E+012 0.000
6000.0

!REF:PITZ ESTIMATE
C2H3OOH<=>CH2CHO+OH 8.400E+014 0.000
43000.0

!REF:!FLOWERS, M. C., J. CHEM. SOC. FAR. TRANS. I 73, 1927 (1977)
C3H6O1-2<=>C2H4+CH2O 6.000E+014 0.000
60000.0

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

!REF:WESTBROOK AND PITZ ESTIMATE (1983)
C3H6O1-3<=>C2H4+CH2O 6.000E+014 0.000
60000.0

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

!REF:
NC3H7O2<=>C3H6+HO2 4.308E+036 -7.500
39510.0

!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) 1.355E+037 -6.036
92929.0
LOW/ 4.720E+018 0.000
49578.0/
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) 6.600E+052 -10.626
100330.0
LOW/ 5.340E+017 0.000
42959.0/
TROE/ 9.502E-002 1.000E-020 5.348E+003 4.326E+003/

!REF:
PC4H9+H <=> C4H10 3.610E+013 0.000
0.0
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 17160.0	4.080E+001	3.590
C4H10+HO2<=>SC4H9+H2O2 13720.0	1.264E+002	3.370
!REF:DRYER ESTIMATE		
C4H10+CH3O<=>PC4H9+CH3OH 7000.0	3.000E+011	0.000
C4H10+CH3O<=>SC4H9+CH3OH 7000.0	6.000E+011	0.000
!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=C4H8-1	9.33E+14	-0.54 -232.362
! Kinetics of the reactions of allyl and propargyl radicals with CH3		
!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
C4H8-1+O2<=>C4H71-4+HO2 52290.0	3.000E+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 5884.0	2.700E+004	0.700
C4H8-1+HO2<=>C4H71-4+H2O2 16490.0	2.380E+003	2.550
!REF:TSANG '91		
C4H8-1+CH3O2<=>C4H71-3+CH3O2H 5884.0	2.700E+004	0.700
C4H8-1+CH3O2<=>C4H71-4+CH3O2H 16490.0	2.380E+003	2.550
C4H8-1+CH3O<=>C4H71-3+CH3OH 8609.0	4.000E+001	2.900
C4H8-1+CH3O<=>C4H71-4+CH3OH 6458.0	2.170E+011	0.000
!REF:DECHAUX, J.C., OXID. COMM. 2, 95 (1981)		
C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H 8000.0	1.000E+011	0.000
!C4H8-1+C3H5-A<=>C4H71-3+C3H6 12400.0	7.900E+010	0.000
!REF:ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).		
!C4H71-3+C4H71-3<=>C4H8-1+C4H6 0.0	1.600E+012	0.000
C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H 14900.0	1.400E+012	0.000
C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H 14900.0	1.400E+012	0.000
C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H 14900.0	1.400E+012	0.000
C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H 14900.0	1.400E+012	0.000
C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H 14900.0	1.400E+012	0.000
C4H8-1+CH3O2<=>C4H8O1-2+CH3O 14340.0	1.000E+012	0.000
!REF:ALLARA AND SHAW, 1980, PARALLEL		
H+C4H71-3<=>C4H8-2 0.0	5.000E+013	0.000

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 1.800E+001 2.950
11990.0

!REF:!TWICE RATE OF C3H6+HO2

C4H8-2+C2H5O2<=>C4H71-3+C2H5O2H 3.200E+012 0.000
14900.0
C4H8-2+NC3H7O2<=>C4H71-3+NC3H7O2H 3.200E+012 0.000
14900.0
C4H8-2+IC3H7O2<=>C4H71-3+IC3H7O2H 3.200E+012 0.000
14900.0
C4H8-2+PC4H9O2<=>C4H71-3+PC4H9O2H 3.200E+012 0.000
14900.0
C4H8-2+SC4H9O2<=>C4H71-3+SC4H9O2H 3.200E+012 0.000
14900.0

!REF:ANALOGY TO C3H6+HO2

C4H8-1+HO2<=>C4H8O1-2+OH 1.000E+012 0.000
14340.0

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

!REF:SEATTLE, AUGUST, 1988

C4H8-2+HO2<=>C4H8O2-3+OH 5.620E+011 0.000
12310.0
C4H8-2+CH3O2<=>C4H8O2-3+CH3O 5.620E+011 0.000
12310.0

!REF:TULLY, PRIVATE COMMUNICATION, 1986.

C4H8-1+OH<=>PC4H8OH 4.750E+012 0.000
-782.0
C4H8-2+OH<=>SC4H8OH 4.750E+012 0.000
-782.0
PC4H8OH+O2<=>C4H8OH-1O2 2.000E+012 0.000
0.0
SC4H8OH+O2<=>C4H8OH-2O2 2.000E+012 0.000
0.0

!REF:ANALOGY TO PROPENE

C4H8OH-1O2=>C2H5CHO+CH2O+OH 1.000E+016 0.000
25000.0

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				5.700E+036	-6.270
112353.0					
C4H6<=>C4H5-N+H				5.300E+044	-8.620
123608.0					
C4H6<=>C4H4+H2				2.500E+015	0.000
94700.0					
!C4H6+H<=>C4H5-N+H2				1.330E+006	2.530
12240.0					
!C4H6+H<=>C4H5-I+H2				6.650E+005	2.530
9240.0					
!C4H6+H<=>C2H4+C2H3				1.460E+030	-4.340
21647.0					
!PLOG/	1.0000	1.460E+030	-4.340	21647.0/	
!PLOG/	10.0000	5.450E+030	-4.510	21877.0/	
C4H6+H<=>C3H4-P+CH3				2.000E+012	0.000
7000.0					
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 0.0	2.000E+012	0.000
C4H5-N+HCO<=>C4H6+CO 0.0	5.000E+012	0.000
C4H5-N+HO2=>C2H3+CH2CO+OH 0.0	6.600E+012	0.000
C4H5-N+H2O2<=>C4H6+HO2 -596.0	1.210E+010	0.000
C4H5-N+HO2<=>C4H6+O2 0.0	6.000E+011	0.000
C4H5-N+O2<=>CH2CHCHCHO+O 11.0	3.000E+011	0.290
C4H5-N+O2<=>HCO+C2H3CHO 1010.0	9.200E+016	-1.390
C4H5-I+H<=>C4H4+H2 0.0	3.000E+013	0.000
C4H5-I+H<=>C3H3+CH3 2000.0	2.000E+013	0.000
C4H5-I+OH<=>C4H4+H2O 0.0	4.000E+012	0.000
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				3.000E+013	0.000
65000.0					
C4H6-2<=>C4H612				3.000E+013	0.000
67000.0					
C4H6-2+H<=>C4H612+H				2.000E+013	0.000
4000.0					
C4H6-2+H<=>C4H5-2+H2				3.400E+005	2.500
2490.0					
C4H6-2+H<=>CH3+C3H4-P				2.600E+005	2.500
1000.0					
C4H6-2<=>H+C4H5-2				5.000E+015	0.000
87300.0					
C4H6-2+CH3<=>C4H5-2+CH4				1.400E+014	0.000
18500.0					
C2H3CHOCH2<=>C4H6O23				2.000E+014	0.000
50600.0					
C4H6O23<=>CH3CHCHCHO				1.950E+013	0.000
49400.0					
C4H6O23<=>C2H4+CH2CO				5.750E+015	0.000
69300.0					
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				2.500E+013	0.000
0.0					
C3H3+CH<=>C4H3-I+H				5.000E+013	0.000
0.0					
C3H3+CH2<=>C4H4+H				5.000E+013	0.000
0.0					
C3H3+CH3 (+M) <=>C4H612 (+M)				1.500E+012	0.000
0.0					
LOW/				2.600E+057	-11.940
9770.0/					
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)				8.300E+010	0.899
-363.0					
LOW/				1.240E+031	-4.718
1871.0/					
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				4.100E+043	-9.490
53000.0					
C4H3-N+H<=>C4H3-I+H				2.500E+020	-1.670
10800.0					
C4H3-N+H<=>C2H2+H2CC				6.300E+025	-3.340
10014.0					
C4H3-N+H<=>C4H4				2.000E+047	-10.260
13070.0					
C4H3-N+H<=>C4H2+H2				3.000E+013	0.000
0.0					
C4H3-N+OH<=>C4H2+H2O				2.000E+012	0.000
0.0					
C2H2+C2H (+M) <=>C4H3-I (+M)				8.300E+010	0.899
-363.0					
LOW/				1.240E+031	-4.718
1871.0/					
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	2.800E+023	-2.550
10780.0		
C4H3-I+H<=>C4H4	3.400E+043	-9.010
12120.0		
C4H3-I+H<=>C4H2+H2	6.000E+013	0.000
0.0		
C4H3-I+OH<=>C4H2+H2O	4.000E+012	0.000
0.0		
C4H3-I+O2<=>HCCO+CH2CO	7.860E+016	-1.800
0.0		
!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)		
C4H3-I+CH2<=>C3H4-A+C2H	2.000E+013	0.000
0.0		
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C2H2+C2H<=>C4H2+H	9.600E+013	0.000
0.0		
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 0.0	5.000E+012	0.000
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
C4H8O1-4+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O1-4+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O1-4+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O1-4+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
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 42500.0	1.500E+016	0.000
 !REF:PITZ ESTIMATE		
SC4H9O+OH<=>SC4H9O2H 0.0	1.000E+015	-0.800
 !REF:		
NC3H7+CH2O<=>PC4H9O 3457.0	5.000E+010	0.000
CH3+C2H5CHO<=>SC4H9O 9043.0	5.000E+010	0.000
C2H5+CH3CHO<=>SC4H9O 6397.0	3.330E+010	0.000
 !REF:		
PC4H9O2<=>C4H8OOH1-2 31850.0	2.000E+011	0.000
PC4H9O2<=>C4H8OOH1-3 20850.0	2.500E+010	0.000
PC4H9O2<=>C4H8OOH1-4 22350.0	4.688E+009	0.000
SC4H9O2<=>C4H8OOH2-1 34500.0	3.000E+011	0.000
SC4H9O2<=>C4H8OOH2-3 31850.0	2.000E+011	0.000
SC4H9O2<=>C4H8OOH2-4 24400.0	3.750E+010	0.000
PC4H9O2<=>C4H8-1+HO2 39510.0	4.308E+036	-7.500
SC4H9O2<=>C4H8-1+HO2 41530.0	5.980E+042	-9.430
SC4H9O2<=>C4H8-2+HO2 39510.0	4.308E+036	-7.500

!REF:

C4H8-1+HO2<=>C4H8OOH1-2 11000.0	1.000E+011	0.000
C4H8-1+HO2<=>C4H8OOH2-1 11750.0	1.000E+011	0.000
C4H8-2+HO2<=>C4H8OOH2-3 11750.0	1.000E+011	0.000
!REF:GREEN 2003		
C4H8OOH1-2<=>C4H8O1-2+OH 15900.0	1.380E+012	0.000
C4H8OOH1-3<=>C4H8O1-3+OH 19500.0	2.040E+011	0.000
C4H8OOH1-4<=>C4H8O1-4+OH 14800.0	5.130E+010	0.000
C4H8OOH2-1<=>C4H8O1-2+OH 17000.0	3.980E+012	0.000
C4H8OOH2-3<=>C4H8O2-3+OH 15900.0	1.380E+012	0.000
C4H8OOH2-4<=>C4H8O1-3+OH 21900.0	4.470E+011	0.000
!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 1.250E+010 0.000
17850.0

!REF:

NC4KET12=>C2H5CHO+HCO+OH 1.050E+016 0.000
41600.0

NC4KET13=>CH3CHO+CH2CHO+OH 1.050E+016 0.000
41600.0

NC4KET14=>CH2CH2CHO+CH2O+OH 1.500E+016 0.000
42000.0

NC4KET21=>CH2O+C2H5CO+OH 1.500E+016 0.000
42000.0

NC4KET23=>CH3CHO+CH3CO+OH 1.050E+016 0.000
41600.0

NC4KET24=>CH2O+CH3COCH2+OH 1.500E+016 0.000
42000.0

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

C2H5COCH3+OH<=>CH2CH2COCH3+H2O 7.550E+009 0.970
1586.0

!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 2.050E+013 0.000
49150.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+CH3<=>CH2CH2COCH3+CH4 3.190E+001 3.170
7172.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+CH3<=>CH3CHCOCH3+CH4 1.740E+000 3.460
3680.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995
C2H5COCH3+CH3<=>C2H5COCH2+CH4 1.620E+011 0.000
9630.0

!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995
C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH 2.170E+011 0.000
6460.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH 1.450E+011 0.000
2771.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH 2.170E+011 0.000
4660.0

!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995
C2H5COCH3+CH3O2<=>CH2CH2COCH3+CH3O2H 3.010E+012 0.000
19380.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+CH3O2<=>CH3CHCOCH3+CH3O2H 2.000E+012 0.000
15250.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL
(C<=>O); CURRAN 1995
C2H5COCH3+CH3O2<=>C2H5COCH2+CH3O2H 3.010E+012 0.000
17580.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+C2H3<=>CH2CH2COCH3+C2H4 5.000E+011 0.000
10400.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+C2H3<=>CH3CHCOCH3+C2H4 3.000E+011 0.000
3400.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995
C2H5COCH3+C2H3<=>C2H5COCH2+C2H4 6.150E+010 0.000
4278.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995
C2H5COCH3+C2H5<=>CH2CH2COCH3+C2H6 5.000E+010 0.000
13400.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+C2H5<=>CH3CHCOCH3+C2H6 3.000E+010 0.000
8600.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);
CURRAN 1995
C2H5COCH3+C2H5<=>C2H5COCH2+C2H6 5.000E+010 0.000
11600.0

!REF: CURRAN AND GAFFURI, 1995
CH3CHCOCH3+O2<=>CH3CHOOCH3 1.000E+011 0.000
0.0
CH3CHOOCH3<=>CH2CHOOHCOCH3 8.900E+012 0.000
29700.0
C2H3COCH3+HO2<=>CH2CHOOHCOCH3 7.000E+010 0.000
7800.0

!REF:
CH2CH2COCH3<=>C2H4+CH3CO 1.000E+014 0.000
18000.0

!REF: WKM 19/ 04/ 2010
C2H5COCH2<=>CH2CO+C2H5 1.000E+014 0.000
35000.0

!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS
C2H3COCH3+H<=>CH3CHCOCH3 5.000E+012 0.000
1200.0

!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS
CH3CHCO+CH3<=>CH3CHCOCH3 1.230E+011 0.000
7800.0

!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 10200.0	4.090E+004	2.500
!REF:CURRAN ESTIMATE		
NC3H7CHO+OH<=>C3H6CHO-1+H2O 1586.0	5.280E+009	0.970
NC3H7CHO+OH<=>C3H6CHO-2+H2O -35.0	4.680E+007	1.610
NC3H7CHO+OH<=>C3H6CHO-3+H2O -1176.0	5.520E+002	3.120
NC3H7CHO+HO2<=>C3H6CHO-1+H2O2 16490.0	2.379E+004	2.550
NC3H7CHO+HO2<=>C3H6CHO-2+H2O2 13910.0	9.640E+003	2.600
NC3H7CHO+HO2<=>C3H6CHO-3+H2O2 17880.0	3.440E+012	0.050
!REF:CURRAN ESTIMATE		
NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H 16490.0	2.379E+004	2.550
NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H 13910.0	9.640E+003	2.600
NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H 17880.0	3.440E+012	0.050
NC3H7CO<=>NC3H7+CO 9600.0	1.000E+011	0.000
!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95.		
C3H6CHO-1<=>C2H4+CH2CHO 21970.0	7.400E+011	0.000
!REF:CURRAN ESTIMATE		
C2H5CHCO+H<=>C3H6CHO-3 1200.0	5.000E+012	0.000
C2H3CHO+CH3<=>C3H6CHO-3 7800.0	1.230E+011	0.000
SC3H5CHO+H<=>C3H6CHO-2 2900.0	5.000E+012	0.000

C3H6+HCO<=>C3H6CHO-2 6000.0	1.000E+011	0.000
C2H5CHCO+OH<=>NC3H7+CO2 -1010.0	3.730E+012	0.000
C2H5CHCO+H<=>NC3H7+CO 1459.0	4.400E+012	0.000
C2H5CHCO+O<=>C3H6+CO2 -437.0	3.200E+012	0.000
!REF:ANALOGY WITH ACETALDEHYDE		
SC3H5CHO+OH<=>SC3H5CO+H2O -340.0	2.690E+010	0.760
!REF:PITZ ESTIMATE		
C3H5-S+CO<=>SC3H5CO 8000.0	5.000E+012	0.000
!REF:ANALOGY WITH IC3H5CHO+X --> IC3H5CO+HX		
SC3H5CHO+HO2<=>SC3H5CO+H2O2 11920.0	1.000E+012	0.000
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
!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
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:		
IC4H9+O2<=>IC4H9O2	2.260E+012	0.000
0.0		
TC4H9+O2<=>TC4H9O2	1.410E+013	0.000
0.0		

!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
!REF:WESTBROOK ESTIMATE		
TC4H9O2+CH4<=>TC4H9O2H+CH3 20460.0	1.130E+013	0.000
!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
TC4H9O2+IC4H7<=>TC4H9O+IC4H7O -1000.0	7.000E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C2H4<=>IC4H9O2H+C2H3 6000.0	2.000E+011	0.000
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
5860.0 1.000E+012 0.000

CH2O+IC3H7<=>IC4H9O
2330.0 5.000E+010 0.000

CH3COCH3+CH3<=>TC4H9O
11900.0 1.500E+011 0.000

!REF:!ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503 (1985).

IC4H9O+O2<=>IC3H7CHO+HO2
1660.0 1.930E+011 0.000

!REF:PITZ ESTIMATE

TC4H9O+O2<=>IC4H8O+HO2
4700.0 8.100E+011 0.000

!REF:FLOWERS, M.C.; PARKER, R.M. INTL. J. CHEM. KINET. 443-452, 1971.

!REF: X 2.0

IC4H8O<=>IC3H7CHO
52720.0 4.180E+013 0.000

!REF:

IC4H8O+OH<=>IC3H6CHO+H2O
0.0 1.250E+012 0.000

IC4H8O+H<=>IC3H6CHO+H2
0.0 1.250E+012 0.000

IC4H8O+HO2<=>IC3H6CHO+H2O2
15000.0 2.500E+012 0.000

IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H
19000.0 2.500E+012 0.000

IC4H8O+CH3<=>IC3H6CHO+CH4
10000.0 5.000E+010 0.000

IC4H8O+O<=>IC3H6CHO+OH
0.0 1.250E+012 0.000

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES

TC3H6CHO+H<=>IC3H7CHO 0.0	2.000E+014	0.000
!REF:TSANG J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
IC3H7+HCO<=>IC3H7CHO 0.0	1.810E+013	0.000
!REF:		
IC3H7CHO+HO2<=>IC3H7CO+H2O2 11920.0	3.000E+012	0.000
!REF:BALDWIN, R.R.; WALKER, R.W.		
!REF:SYMP. INTL. COMB. PROC. 1979, 17, 525.		
IC3H7CHO+HO2<=>TC3H6CHO+H2O2 11920.0	8.000E+010	0.000
!REF:BIRRELL, R.N.; TROTMAN-DICKENSON, A.F. J. CHEM. SOC. 1960, 2059		
IC3H7CHO+CH3<=>IC3H7CO+CH4 8700.0	3.980E+012	0.000
!REF:SINGLETON, D.L. ET AL. CAN. J. CHEM. 1977, 55, 3321.		
IC3H7CHO+O<=>IC3H7CO+OH 1389.0	7.180E+012	0.000
!REF: BALDWIN, R.R. ET AL. J. CHEM. SOC. FAR. TRANS. 1979, 75, 1433		
IC3H7CHO+O2<=>IC3H7CO+HO2 37600.0	4.000E+013	0.000
!REF:SEMMES ET AL. INTL. J. CHEM. KINET. 1985, 17, 303.		
IC3H7CHO+OH<=>IC3H7CO+H2O -340.0	2.690E+010	0.760
IC3H7CHO+OH<=>TC3H6CHO+H2O -781.0	1.684E+012	0.000
!REF: CURRAN ESTIMATE		
IC3H7CHO+H<=>IC3H7CO+H2 2600.0	2.600E+012	0.000
IC3H7CHO+OH<=>IC3H6CHO+H2O -298.0	3.120E+006	2.000
IC3H7CHO+HO2<=>IC3H6CHO+H2O2 15500.0	2.740E+004	2.550
IC3H7CHO+CH3O2<=>IC3H6CHO+CH3O2H 16490.0	4.760E+004	2.550
!REF:NAROZNIK, M; NIEDZIELSKI, J. J. PHOTOCHEM. 1986, 32, 281		
IC3H7+CO<=>IC3H7CO 4810.0	1.500E+011	0.000
!REF:CURRAN ESTIMATE		
C3H6+HCO<=>IC3H6CHO 7800.0	1.000E+011	0.000
C2H3CHO+CH3<=>IC3H6CHO 7800.0	1.000E+011	0.000
!REF:		
IC4H8+OH<=>IC4H8OH -960.0	9.930E+011	0.000

IC4H8OH+O2<=>IO2C4H8OH -1100.0	1.200E+011	0.000
IO2C4H8OH=>CH3COCH3+CH2O+OH 18900.0	1.250E+010	0.000
IC4H9O2<=>IC4H8O2H-I 24400.0	7.500E+010	0.000
TC4H9O2<=>TC4H8O2H-I 34500.0	9.000E+011	0.000
IC4H9O2<=>IC4H8O2H-T 29200.0	1.000E+011	0.000
IC4H9O2<=>IC4H8+HO2 39490.0	2.265E+035	-7.220
TC4H9O2<=>IC4H8+HO2 41490.0	7.612E+042	-9.410
!REF:		
IC4H8O2H-I+O2<=>IC4H8OOH-IO2 0.0	2.260E+012	0.000
TC4H8O2H-I+O2<=>TC4H8OOH-IO2 0.0	2.260E+012	0.000
IC4H8O2H-T+O2<=>IC4H8OOH-TO2 0.0	1.410E+013	0.000
!REF:		
IC4H8OOH-IO2<=>IC4KETII+OH 21400.0	5.000E+010	0.000
IC4H8OOH-TO2<=>IC4KETIT+OH 31500.0	4.000E+011	0.000
TC4H8OOH-IO2<=>TIC4H7Q2-I 24400.0	7.500E+010	0.000
!REF:CURRAN ESTIMATE		
IC4H7OOH+HO2<=>TIC4H7Q2-I 10600.0	1.000E+011	0.000
!REF:		
IC4H8OOH-IO2<=>IIC4H7Q2-I 24400.0	3.750E+010	0.000
IC4H8OOH-IO2<=>IIC4H7Q2-T 29200.0	1.000E+011	0.000
IC4H8OOH-TO2<=>TIC4H7Q2-I 34500.0	6.000E+011	0.000
!REF:CURRAN ESTIMATE		
AC3H5OOH+CH2O2H<=>IIC4H7Q2-I 10600.0	8.500E+010	0.000
IC4H7OOH+HO2<=>IIC4H7Q2-T 7800.0	1.000E+011	0.000
CH2O2H<=>CH2O+OH 1500.0	9.000E+014	0.000
IC4KETII=>CH2O+C2H5CO+OH 42000.0	1.500E+016	0.000
IC4KETIT=>CH3COCH3+HCO+OH 42540.0	9.500E+015	0.000
!REF:		
IC4H8+HO2<=>TC4H8O2H-I 12620.0	3.970E+011	0.000

IC4H8+HO2<=>IC4H8O2H-T 12620.0	3.970E+011	0.000
!REF:GREEN 2003		
IC4H8O2H-I<=>CC4H8O+OH 21900.0	4.470E+011	0.000
IC4H8O2H-T<=>IC4H8O+OH 13400.0	3.090E+012	0.000
TC4H8O2H-I<=>IC4H8O+OH 17000.0	3.980E+012	0.000
!REF:		
IC4H8O2H-I=>OH+CH2O+C3H6 29170.0	8.451E+015	-0.680
IC4H8<=>C3H5-T+CH3 128100.0	1.920E+066	-14.220
IC4H8<=>IC4H7+H 114300.0	3.070E+055	-11.490
IC4H8+H<=>C3H6+CH3 20000.0	5.680E+033	-5.720
!REF:ANALOGY WITH TSANG '92: C3H6+R<=>PRODUCTS		
IC4H8+H<=>IC4H7+H2 2492.0	3.400E+005	2.500
!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:		
IC4H8+CH3<=>IC4H7+CH4 5675.0	4.420E+000	3.500
IC4H8+HO2<=>IC4H7+H2O2 13910.0	1.928E+004	2.600
!REF:ANALOGY WITH RH+RO2 --> R+RO2H		
IC4H8+O2CHO<=>IC4H7+HO2CHO 13910.0	1.928E+004	2.600
!REF:		
IC4H8+O2<=>IC4H7+HO2 39900.0	6.000E+012	0.000
!REF:WESTBROOK AND PITZ ESTIMATE 1983		
IC4H8+C3H5-A<=>IC4H7+C3H6 20500.0	7.940E+011	0.000
IC4H8+C3H5-S<=>IC4H7+C3H6 20500.0	7.940E+011	0.000
IC4H8+C3H5-T<=>IC4H7+C3H6 20500.0	7.940E+011	0.000

IC4H8+OH<=>IC4H7+H2O -298.0	5.200E+006	2.000
IC4H8+O<=>IC3H7+HCO -1216.0	1.580E+007	1.760
!REF:		
IC4H8+CH3O2<=>IC4H7+CH3O2H 13910.0	1.928E+004	2.600
!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 BOZZELLI C3H5-A+O2 @ 10 ATM		
IC4H7+O2<=>IC3H5CHO+OH 23020.0	2.470E+013	-0.450
IC4H7+O2<=>CH3COCH2+CH2O 21050.0	7.140E+015	-1.210
IC4H7+O2=>C3H4-A+CH2O+OH 21450.0	7.290E+029	-5.710
!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: ANALOGY C3H5-A+X --> PRODUCTS		
IC4H6OH+H2<=>IC4H7OH+H 18990.0	2.160E+004	2.380
!REF:		
IC4H7OH+O2<=>IC4H6OH+HO2 39900.0	6.000E+013	0.000
!REF: RATE CONSTANT ANALOGY TO C3H5-A+CH2O (X 5)		
IC4H6OH+CH2O<=>IC4H7OH+HCO 18190.0	6.300E+008	1.900
!REF: CURRAN ESTIMATE		
IC4H6OH+IC4H8<=>IC4H7OH+IC4H7 19840.0	4.700E+002	3.300
IC4H6OH+H<=>IC4H7OH 0.0	1.000E+014	0.000

IC4H6OH+H2O2<=>IC4H7OH+HO2 13580.0	7.830E+005	2.050
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+H2O 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:ANALOGOUS TO ISOBUTERALDEHYDE+X		
IC3H5CHO+HO2<=>IC3H5CO+H2O 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:		
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:ANALOGY WITH C3H5-A+CH3 --> 1-C4H8 TSANG 91 (PROPENE).		
TC3H6OCHO+OH<=>TC3H6CHO+HO2 21010.0	2.018E+017	-1.200
!REF:CURRAN AND GAFFURI, 1995.		
TC3H6OCHO<=>CH3COCH3+HCO 9700.0	3.980E+013	0.000
!REF:		
IC3H5CHO+H<=>TC3H6CHO 1200.0	1.300E+013	0.000
IC3H6CO+H<=>TC3H6CHO 4800.0	1.300E+013	0.000

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES		
TC3H6CHO+H2<=>IC3H7CHO+H 18990.0	2.160E+005	2.380
IC4H7O+OH<=>IC4H7OOH 0.0	1.000E+011	0.000
IC4H7O+H<=>IC4H7OH 0.0	4.000E+013	0.000
!REF:ANALOGY WITH IC4H9 --> IC4H8+H		
IC4H7OH+H<=>IC4H8OH 1200.0	1.000E+013	0.000
!REF:ANALOGY WITH HCO+H2 --> CH2O+H		
!REF:(TSANG/ HAMPSON 86) X 5		
IC4H7O+H2<=>IC4H7OH+H 17830.0	9.050E+006	2.000
!REF:CURRAN ESTIMATE		
IC4H7+OH<=>IC4H7OH 0.0	3.000E+013	0.000
IC4H7OH+HCO<=>IC4H7O+CH2O 18160.0	3.020E+011	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:		
TC3H6O2HCO=>CH3COCH3+CO+OH 4800.0	4.244E+018	-1.430
!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

!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 1.320E+002 3.250
5590.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
C6H5=>H+C4H2+C2H2 4.300E+012 0.620
77294.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
C6H5+CH2O<=>C6H6+HCO 8.550E+004 2.190
38.0

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

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
C6H5+HCO<=>C6H6+CO 8.550E+004 2.190
38.0

!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003
C6H5+HO2<=>C6H5O+OH 5.000E+012 0.000
0.0

!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.
C6H5+O2<=>C6H5O+O 2.600E+013 0.000
6120.0

!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.
C6H5+O2<=>O-C6H4O2+H 3.000E+013 0.000
8980.0

!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575
C6H5+O2<=>C6H5OO 1.860E+013 -0.220
-711.0

!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575
C6H5OO<=>C6H5O+O 1.270E+015 -0.246
38536.0

!REF:WKM ESTIMATED
C6H5O+OH<=>C6H5OOH 2.000E+013 0.000
0.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
C6H5OO+C6H5OH<=>C6H5OOH+C6H5O 1.330E+011 0.000
14000.0

!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003
C6H5OH+O2<=>C6H5O+HO2 1.000E+013 0.000
38800.0
C6H5OH+O<=>OC6H4OH+H 1.600E+013 0.000
3400.0

C6H5OH+H<=>C6H5O+H2	1.200E+014	0.000
12400.0		
C6H5OH+O<=>C6H5O+OH	1.300E+013	0.000
2900.0		
C6H5OH+OH<=>C6H5O+H2O	1.400E+008	1.400
-960.0		
C6H5OH+HO2<=>C6H5O+H2O2	1.000E+012	0.000
10000.0		
C6H5OH+CH3<=>C6H5O+CH4	1.800E+011	0.000
7700.0		
C6H5OH+C6H5<=>C6H5O+C6H6	4.900E+012	0.000
4400.0		
C6H5OH+C3H5-A<=>C6H5O+C3H6	4.900E+011	0.000
9400.0		
C6H5OH+C4H5-I<=>C6H5O+C4H6	4.900E+011	0.000
9400.0		
C6H5OH+H<=>C6H4OH+H2	1.700E+014	0.000
16000.0		
C6H5OH+O<=>C6H4OH+OH	2.000E+013	0.000
14700.0		
C6H5OH+OH<=>C6H4OH+H2O	1.400E+013	0.000
4600.0		
C6H5OH+HO2<=>C6H4OH+H2O2	4.000E+011	0.000
28900.0		
C6H5OH+CH3<=>C6H4OH+CH4	2.000E+012	0.000
15000.0		
C6H4OH+O2<=>OC6H4OH+O	2.100E+013	0.000
6100.0		
C6H4OH+H<=>C6H5OH	1.000E+014	0.000
0.0		
OC6H4OH<=>C5H4OH+CO	7.400E+011	0.000
43800.0		

!REF:WKM REDUCED FROM 2.5E+14

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

C6H5O+H(+M)<=>C6H5OH(+M)	2.000E+014	0.000
0.0		
LOW/	1.000E+094	-21.840
13880.0/		
TROE/ 4.300E-002 3.042E+002 6.000E+004 5.896E+003/		

!REF:XU AND LIN J PHYS CHEM 110 1672-1677 2006

!REF:WKM A FACTOR *0.5 TO FIT PYROLYSIS DATA

C6H5OH<=>C5H6+CO	4.310E+015	-0.610
74115.0		

!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	2.000E+011	0.000
43900.0		

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)
 2007
 C6H5O+H<=>CO+C5H6 1.000E+013 0.000
 0.0
 C6H5O+O<=>C5H5+CO2 1.000E+013 0.000
 0.0
 C6H5O+O<=>OC6H4OH 2.600E+010 0.470
 800.0

!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 2.000E+012 0.000
 0.0

!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38:
 250-275, 2006
 P-C6H4O2+H<=>P-OC6H5OJ 4.000E+012 0.000
 9740.0

!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38:
 250-275, 2006
 O-C6H4O2+H<=>O-OC6H5OJ 4.000E+012 0.000
 6960.0

!REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
 C6H5O+O<=>P-C6H4O2+H 4.250E+013 0.000
 0.0
 C6H5O+O<=>O-C6H4O2+H 8.500E+013 0.000
 0.0
 O-C6H4O2<=>C5H4O+CO 1.000E+012 0.000
 40000.0
 P-C6H4O2<=>C5H4O+CO 3.700E+011 0.000
 59000.0
 P-C6H4O2+H<=>C5H5O+CO 2.500E+013 0.000
 4700.0
 P-C6H4O2+H<=>P-C6H3O2+H2 2.000E+012 0.000
 8100.0
 P-C6H4O2+O<=>P-C6H3O2+OH 1.400E+013 0.000
 14700.0
 P-C6H4O2+OH<=>P-C6H3O2+H2O 1.000E+006 2.000
 4000.0
 P-C6H3O2+H<=>P-C6H4O2 1.000E+014 0.000
 0.0
 P-C6H3O2+H<=>2C2H2+2CO 1.000E+014 0.000
 0.0
 P-C6H3O2+O=>C2H2+HCCO+2CO 1.000E+014 0.000
 0.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)
 2007
 P-C6H4O2+O=>2CO+C2H2+CH2CO 3.000E+013 0.000
 5000.0
 C5H5+H (+M) <=>C5H6 (+M) 2.600E+014 0.000
 0.0

LOW/ 4.400E+080 -18.280
 12994.0/
 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) 3.800E+017 0.000
 104000.0
 LOW/ 1.000E+098 -22.250
 126321.5/
 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 4.000E+013 0.000
 37150.0
 C5H6+HO2<=>C5H5+H2O2 1.100E+004 2.600
 12900.0
 C5H6+OH<=>C5H5+H2O 3.080E+006 2.000
 0.0

!REF:ROY AND FRANK, 21ST INTERNATIONAL SYMPOSIUM ON SHOCKWAVES, 1997 PPER
 1560
 !C5H6+H<=>C5H5+H2 7.200E+013 0.000
 3500.0

!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998
 !C5H6+H<=>C2H2+C3H5-A 1.548E+037 -6.180
 32890.0
 C5H6+O<=>C5H5+OH 4.800E+004 2.710
 1100.0
 C5H6+C2H3<=>C5H5+C2H4 1.200E-001 4.000
 0.0

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
 C5H6+C6H5O<=>C5H5+C6H5OH 3.160E+011 0.000
 8000.0

!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998
 !C5H6+CH3<=>C5H5+CH4 1.800E-001 4.000
 0.0

!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998
 C5H6+C6H5<=>C5H5+C6H6 1.000E-001 4.000
 0.0

!REF:ON OTHER CONDITIONS.
 !C5H6+C5H5<=>C6H6+C4H5-N 5.000E+009 0.000
 0.0

!REF:LIN J COMPUT CHEM 21 415-425 2000
 C5H5<=>C3H3+C2H2 1.980E+068 -15.000
 124900.0

!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 -860.0	3.000E+008	1.450
C4H4O+OH<=>C3H5-A+CO2 0.0	3.000E+012	0.000
!REF:LIN J COMPUT CHEM 21 415-425 2000		
C3H3+C2H2<=>C#CC*CCJ 45400.0	4.110E+072	-18.200
C#CC*CCJ<=>C5H5 34058.3	8.000E+013	0.000
C#CC*CCJ+H<=>C5H6 0.0	1.000E+014	0.000
!REF:LINDSTEDT C&F 99:551-561 (1994)		
C#CC*CCJ+H<=>C5H6-L 0.0	1.000E+010	0.000
C5H6-L+O<=>C#CC*CCJ+OH 0.0	1.000E+010	0.000
C5H6-L+OH<=>C#CC*CCJ+H2O 0.0	1.000E+010	0.000

!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	3.000E+013	0.000
43710.0		
CJ*CC*O<=>C2H3CO	1.400E+009	0.980
32100.0		
C2H2+HCO<=>CJ*CC*O	7.770E+006	1.410
7755.0		

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

C5H4OH+H<=>C5H5OH	1.000E+014	0.000
0.0		
C5H4OH+H<=>C5H4O+H2	2.100E+013	0.000
54000.0		
C5H4OH+O2<=>C5H4O+HO2	3.000E+013	0.000
5000.0		

!REF:WANG AND BREZINSKY J PHYS CHEM A 102: 1530 1998

C5H4O=>CO+C2H2+C2H2	5.700E+032	-6.760
68500.0		
DUP		
C5H4O=>CO+C2H2+C2H2	6.200E+041	-7.870
98700.0		

DUP

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

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C5H4O+H<=>C4H5-N+CO 2.100E+061 -13.270
40810.0

!REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.

C5H4O+O<=>C4H4+CO2 1.000E+013 0.000
2000.0
C5H4O+H<=>C5H3O+H2 2.000E+012 0.000
8100.0
C5H4O+O<=>C5H3O+OH 1.400E+013 0.000
1470.0
C5H4O+OH<=>C5H3O+H2O 1.100E+008 1.420
1450.0
C5H3O+H<=>C5H4O 1.000E+014 0.000
0.0

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

C5H3O+O2=>CO2+C2H2+HCCO 9.700E+058 -13.470
38180.0
C5H3O=>C2H2+CO+C2H 2.000E+013 0.000
51000.0

!REF:ARENDS ET AL. J PHYS CHEM 97: 7914 1993

!C5H7<=>C*CCJC*C 3.200E+015 0.000
39500.0

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

C5H7+H<=>C5H6+H2 3.600E+012 0.000
0.0
C5H7+O<=>C5H6+OH 1.000E+013 0.000
0.0

!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 9530.0	1.300E+015	-1.070
C5H6+HCO<=>C5H5+CH2O 16000.0	1.080E+008	1.900
C5H6+C2H3<=>C6H6+CH3 42460.0	2.100E+067	-16.080
!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
!C5H6+C4H5-I<=>C5H5+C4H6 0.0	6.000E+012	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
!C*CCJC*C<=>C*CC*CCJ 60.0	5.400E+011	-0.700
!C*CC*CCJ+H<=>C*CC*CC 3020.0	2.300E+020	-1.600
!C*CC*CC+H<=>C4H6+CH3 51000.0	5.200E+071	-16.380
!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996		
!C*CC*CC+H<=>C*CC*CCJ+H2 5000.0	7.000E+006	2.000
!C*CC*CC+OH<=>C*CC*CCJ+H2O 0.0	7.000E+006	2.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
!C*CCJC*C+O2<=>C2H3CHO+CH2CHO 33600.0	1.200E+036	-7.250
C*CC*CCJ+O2<=>C2H3CHO+CH2CHO 33600.0	1.200E+036	-7.250
C*CC*CCJ+H<=>C4H5-N+CH3 36770.0	2.900E+026	-2.180
!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996		
!C*CCJC*C+O<=>C2H3CHO+C2H3 0.0	2.000E+014	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C*CC*CCJ+OH<=>C*CC*CCOH 0.0	1.500E+013	0.000
C*CC*CCJ+O2<=>C*CCJC*O+CH2O 9140.0	8.200E+010	0.180
C*CC*CCOH+H<=>C4H6+CH2OH 16250.0	2.500E+034	-6.120
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
OC5H7O+O2<=>OC4H6O+HOCO 33600.0	6.300E+005	-7.250
C*CCJC*COH+O2<=>HOC*CC*O+CH2CHO 33600.0	1.200E+036	-7.250

HOC*CC*O+OH<=>HOC*CCJ*O+H2O -340.0	2.690E+010	0.760
HOC*CC*O+HO2<=>HOC*CCJ*O+H2O2 11920.0	1.000E+012	0.000
HOC*CC*O+CH3<=>HOC*CCJ*O+CH4 8700.0	3.980E+012	0.000
HOC*CC*O+O<=>HOC*CCJ*O+OH 1389.0	7.180E+012	0.000
HOC*CC*O+O2<=>HOC*CCJ*O+HO2 40700.0	2.000E+013	0.000
HOC*CC*O+H<=>HOC*CCJ*O+H2 2600.0	2.600E+012	0.000

!REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO C2H2OH+CO<=>HOC*CCJ*O 4810.0	1.510E+011	0.000
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!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) OC4H6O+H<=>OC4H5O+H2 3279.0	2.300E+010	1.050
OC4H6O+OH<=>OC4H5O+H2O -447.0	3.500E+009	1.180
OC4H5O+O2<=>O2CCHOOJ+C2H4 20670.0	1.600E+045	-9.920
O2CCHOOJ<=>HOCO+CO2 4000.0	3.000E+013	0.000

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

C*CCJC*O<=>C3H5-A+CO -1120.0	6.100E+005	0.920
C*CCJC*O+O2<=>C2H3CHO+HOCO 33600.0	1.200E+036	-7.250

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

HOCO<=>CO+OH 32470.0	6.300E+032	-5.960
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 34240.0	1.897E+038	-8.047
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: Lynch et al. J. Phys. Chem. A, 2013, 117, 4750-4761 DECREASE 30%						
!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						
C2H3+O2=CH2CHOO				4.07E+27		-4.67
5222.0						
PLOG/1.000E-02	1.55E+24		-5.45	9662.0/		
PLOG/1.000E-02	1.78E-09		4.15	-4707.0/		
! fit btw. 400 and 1250 K with MAE of 0.4%, 1.2%						
PLOG/1.000E-01	3.48E+56		-15.01	19160.0/		
PLOG/1.000E-01	2.36E+22		-4.52	2839.0/		
! fit btw. 400 and 1350 K with MAE of 0.2%, 0.5%						
PLOG/3.160E-01	1.25E+64		-16.97	21290.0/		
PLOG/3.160E-01	2.00E+26		-5.43	2725.0/		
! fit btw. 400 and 1450 K with MAE of 0.2%, 0.6%						
PLOG/1.000E+00	3.34E+61		-15.79	20150.0/		
PLOG/1.000E+00	6.13E+28		-5.89	3154.0/		
! fit btw. 400 and 1550 K with MAE of 0.2%, 1.1%						
PLOG/3.160E+00	7.34E+53		-13.11	17300.0/		
PLOG/3.160E+00	2.14E+29		-5.80	3520.0/		
! fit btw. 400 and 1650 K with MAE of 0.3%, 1.5%						
PLOG/1.000E+01	4.16E+48		-11.21	16000.0/		
PLOG/1.000E+01	3.48E+28		-5.37	3636.0/		
! fit btw. 400 and 1750 K with MAE of 0.4%, 1.9%						
PLOG/3.160E+01	2.33E+43		-9.38	14810.0/		

PLOG/3.160E+01 3.32E+27 -4.95 3610.0/
! fit btw. 400 and 1900 K with MAE of 0.6%, 2.5%
PLOG/1.000E+02 3.41E+39 -8.04 14360.0/
PLOG/1.000E+02 1.03E+27 -4.72 3680.0/
! fit btw. 400 and 2100 K with MAE of 0.9%, 3.1%

!C2H3+O2=CHCHO+OH 2.84E+14 -0.80
7232.0

! PLOG/1.000E-02 3.91E+11 -0.11 2131.0/
! PLOG/1.000E-02 9.91E+11 -0.66 -0.6/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
! PLOG/1.000E-01 1.13E+09 0.55 46.0/
! PLOG/1.000E-01 6.94E+14 -1.16 4542.0/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.0%
! PLOG/3.160E-01 8.46E+08 0.56 0.7/
! PLOG/3.160E-01 2.79E+13 -0.72 3479.0/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.1%
! PLOG/1.000E+00 2.75E+14 -1.83 4.6/
! PLOG/1.000E+00 4.99E+11 -0.14 1995.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.3%
! PLOG/3.160E+00 2.58E+20 -2.84 7530.0/
! PLOG/3.160E+00 2.35E+10 0.23 1573.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.3%
! PLOG/1.000E+01 9.18E+14 -2.26 -0.4/
! PLOG/1.000E+01 1.70E+14 -0.82 4450.0/
! fit btw. 400 and 2200 K with MAE of 0.8%, 2.0%
! PLOG/3.160E+01 6.11E+25 -4.21 13050.0/
! PLOG/3.160E+01 1.42E+11 0.05 3774.0/
! fit btw. 400 and 2200 K with MAE of 0.7%, 2.3%
! PLOG/1.000E+02 1.65E+30 -5.35 18430.0/
! PLOG/1.000E+02 3.17E+11 -0.02 5338.0/
! fit btw. 400 and 2200 K with MAE of 1.5%, 5.0%

C2H3+O2=CH2CHO+O 1.60E+12 0.15
4205.0

PLOG/1.000E-02 7.16E+20 -2.67 6742.0/
PLOG/1.000E-02 1.24E+10 0.62 -277.6/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/1.000E-01 7.02E+20 -2.67 6713.0/
PLOG/1.000E-01 1.29E+10 0.62 -247.7/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/3.160E-01 8.97E+20 -2.70 6724.0/
PLOG/3.160E-01 1.51E+10 0.60 -162.5/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00 6.45E+20 -2.65 6489.0/
PLOG/1.000E+00 1.84E+10 0.58 38.4/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/3.160E+00 4.09E+20 -2.53 6406.0/
PLOG/3.160E+00 8.86E+09 0.67 248.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.1%
PLOG/1.000E+01 1.60E+23 -3.22 8697.0/
PLOG/1.000E+01 6.67E+09 0.72 778.1/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.3%
PLOG/3.160E+01 2.85E+25 -3.77 11530.0/
PLOG/3.160E+01 1.43E+09 0.92 1219.0/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.9%
PLOG/1.000E+02 9.28E+25 -3.80 13910.0/

PLOG/1.000E+02 7.14E+07 1.28 1401.0/
! fit btw. 400 and 2200 K with MAE of 0.7%, 2.3%

C2H3+O2=C2H2+HO2 6.49E+06 1.50
5218.0

PLOG/1.000E-02 1.08E+07 1.28 3322.0/
PLOG/1.000E-02 4.76E+01 2.75 -796.4/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.1%
PLOG/1.000E-01 7.75E+06 1.33 3216.0/
PLOG/1.000E-01 5.16E+01 2.73 -768.3/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.1%
PLOG/3.160E-01 1.21E+07 1.27 3311.0/
PLOG/3.160E-01 5.55E+01 2.73 -658.5/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.1%
PLOG/1.000E+00 2.15E+07 1.19 3367.0/
PLOG/1.000E+00 4.60E+01 2.76 -492.8/
! fit btw. 400 and 2200 K with MAE of 0.0%, 0.1%
PLOG/3.160E+00 1.13E+08 1.00 3695.0/
PLOG/3.160E+00 3.75E+00 3.07 -601.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/1.000E+01 1.31E+11 0.12 5872.0/
PLOG/1.000E+01 5.48E+00 3.07 85.7/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.3%
PLOG/3.160E+01 1.19E+09 0.82 5617.0/
PLOG/3.160E+01 4.47E+08 -0.00 955.0/
! fit btw. 400 and 2200 K with MAE of 0.8%, 1.7%
PLOG/1.000E+02 1.06E+17 -1.45 12230.0/
PLOG/1.000E+02 2.02E+01 2.94 1847.0/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.9%

!C2H3+O2=OCHCHO+H 3.08E+12 -
0.26 3277.0

! PLOG/1.000E-02 4.79E+14 -1.03 912.0/
! PLOG/1.000E-02 2.80E-04 4.04 -7019.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/1.000E-01 5.03E+14 -1.04 922.5/
! PLOG/1.000E-01 3.45E-04 4.01 -6978.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/3.160E-01 6.43E+14 -1.07 982.9/
! PLOG/3.160E-01 9.73E-04 3.89 -6768.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/1.000E+00 3.73E+15 -1.29 1441.0/
! PLOG/1.000E+00 4.98E-01 3.15 -5496.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.6%
! PLOG/3.160E+00 2.44E+18 -2.13 3234.0/
! PLOG/3.160E+00 1.34E+05 1.67 -2931.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.8%
! PLOG/1.000E+01 1.30E+15 -1.09 2393.0/
! PLOG/1.000E+01 4.50E+15 -3.08 -4836.0/
! fit btw. 400 and 2200 K with MAE of 1.5%, 3.6%
! PLOG/3.160E+01 3.57E+33 -6.50 14910.0/
! PLOG/3.160E+01 3.84E+10 0.22 941.3/
! fit btw. 400 and 2200 K with MAE of 0.6%, 2.1%
! PLOG/1.000E+02 3.28E+31 -5.76 16250.0/
! PLOG/1.000E+02 2.75E+08 0.83 857.6/
! fit btw. 400 and 2200 K with MAE of 1.0%, 4.0%

C2H3+O2=CH2CO+OH 1.17E+03 2.43
7074.0
PLOG/1.000E-02 8.66E+02 2.41 6061.0/
PLOG/1.000E-02 1.82E-01 3.12 1331.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.7%
PLOG/1.000E-01 8.91E+02 2.41 6078.0/
PLOG/1.000E-01 2.07E-01 3.11 1383.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
PLOG/3.160E-01 9.43E+02 2.40 6112.0/
PLOG/3.160E-01 2.71E-01 3.08 1496.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
PLOG/1.000E+00 1.06E+03 2.39 6180.0/
PLOG/1.000E+00 5.26E-01 3.01 1777.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
PLOG/3.160E+00 1.09E+03 2.38 6179.0/
PLOG/3.160E+00 1.37E+00 2.90 2225.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.4%
PLOG/1.000E+01 1.39E+03 2.36 6074.0/
PLOG/1.000E+01 4.19E-01 2.93 2052.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.2%
PLOG/3.160E+01 2.49E+06 1.42 8480.0/
PLOG/3.160E+01 1.19E-04 4.21 2043.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.3%
PLOG/1.000E+02 1.66E+10 0.36 12010.0/
PLOG/1.000E+02 1.30E-03 3.97 3414.0/
! fit btw. 400 and 2200 K with MAE of 0.1%, 0.5%

! Replace HCO with 70% H + CO
! C2H3+O2=CH2O+HCO 1.29E+16 -1.13
3791.0
! PLOG/1.000E-02 9.24E+36 -7.60 12640.0/
! PLOG/1.000E-02 1.68E+16 -1.28 515.3/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/1.000E-01 8.99E+36 -7.60 12610.0/
! PLOG/1.000E-01 1.70E+16 -1.28 513.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/3.160E-01 7.22E+36 -7.57 12490.0/
! PLOG/3.160E-01 1.78E+16 -1.29 520.6/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%
! PLOG/1.000E+00 1.01E+36 -7.32 11820.0/
! PLOG/1.000E+00 2.25E+16 -1.31 645.7/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.7%
! PLOG/3.160E+00 5.31E+36 -7.47 12460.0/
! PLOG/3.160E+00 3.49E+16 -1.36 1066.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.5%
! PLOG/1.000E+01 1.92E+36 -7.20 13430.0/
! PLOG/1.000E+01 9.48E+15 -1.18 1429.0/
! fit btw. 400 and 2200 K with MAE of 0.4%, 1.9%
! PLOG/3.160E+01 1.18E+21 -2.57 5578.0/
! PLOG/3.160E+01 3.80E+69 -19.23 14760.0/
! fit btw. 400 and 2200 K with MAE of 1.8%, 3.9%
! PLOG/1.000E+02 1.01E+34 -6.28 16000.0/
! PLOG/1.000E+02 1.56E+11 0.19 830.6/
! fit btw. 400 and 2200 K with MAE of 1.8%, 6.8%

C2H3+O2=CH2O+HCO 1.29E+16 -1.13
3791.0
PLOG/1.000E-02 2.77E+36 -7.60 12640.0/

PLOG/1.000E-02	5.04E+15	-1.28	515.3/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/1.000E-01	2.70E+36	-7.60	12610.0/
PLOG/1.000E-01	5.10E+15	-1.28	513.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/3.160E-01	2.17E+36	-7.57	12490.0/
PLOG/3.160E-01	5.34E+15	-1.29	520.6/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/1.000E+00	3.03E+35	-7.32	11820.0/
PLOG/1.000E+00	6.75E+15	-1.31	645.7/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.7%			
PLOG/3.160E+00	1.59E+36	-7.47	12460.0/
PLOG/3.160E+00	1.05E+16	-1.36	1066.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.5%			
PLOG/1.000E+01	5.76E+35	-7.20	13430.0/
PLOG/1.000E+01	2.84E+15	-1.18	1429.0/
! fit btw. 400 and 2200 K with MAE of 0.4%, 1.9%			
PLOG/3.160E+01	3.54E+20	-2.57	5578.0/
PLOG/3.160E+01	1.14E+69	-19.23	14760.0/
! fit btw. 400 and 2200 K with MAE of 1.8%, 3.9%			
PLOG/1.000E+02	3.03E+33	-6.28	16000.0/
PLOG/1.000E+02	4.68E+10	0.19	830.6/
! fit btw. 400 and 2200 K with MAE of 1.8%, 6.8%			

C2H3+O2=>CH2O+H+CO

1.29E+16

-1.13

3791.0

PLOG/1.000E-02	6.47E+36	-7.60	12640.0/
PLOG/1.000E-02	1.18E+16	-1.28	515.3/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/1.000E-01	6.29E+36	-7.60	12610.0/
PLOG/1.000E-01	1.19E+16	-1.28	513.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/3.160E-01	5.05E+36	-7.57	12490.0/
PLOG/3.160E-01	1.25E+16	-1.29	520.6/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/1.000E+00	7.07E+35	-7.32	11820.0/
PLOG/1.000E+00	1.58E+16	-1.31	645.7/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.7%			
PLOG/3.160E+00	3.72E+36	-7.47	12460.0/
PLOG/3.160E+00	2.44E+16	-1.36	1066.0/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.5%			
PLOG/1.000E+01	1.34E+36	-7.20	13430.0/
PLOG/1.000E+01	6.64E+15	-1.18	1429.0/
! fit btw. 400 and 2200 K with MAE of 0.4%, 1.9%			
PLOG/3.160E+01	8.26E+20	-2.57	5578.0/
PLOG/3.160E+01	2.66E+69	-19.23	14760.0/
! fit btw. 400 and 2200 K with MAE of 1.8%, 3.9%			
PLOG/1.000E+02	7.07E+33	-6.28	16000.0/
PLOG/1.000E+02	1.09E+11	0.19	830.6/
! fit btw. 400 and 2200 K with MAE of 1.8%, 6.8%			

C2H3+O2=CO+CH3O

3.09E+13

-0.89

3682.0

PLOG/1.000E-02	8.19E+18	-2.66	3201.0/
PLOG/1.000E-02	1.29E+09	0.18	-1717.0/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.7%			
PLOG/1.000E-01	4.06E+14	-1.32	885.8/

PLOG/1.000E-01	5.99E+11	-2.93	-9564.0/
! fit btw. 400 and 2200 K with MAE of 0.8%, 2.6%			
PLOG/3.160E-01	4.34E+14	-1.33	900.6/
PLOG/3.160E-01	2.91E+11	-2.93	-10120.0/
! fit btw. 400 and 2200 K with MAE of 0.8%, 2.6%			
PLOG/1.000E+00	1.03E+11	-0.33	-747.8/
PLOG/1.000E+00	5.77E+21	-3.54	4772.0/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.7%			
PLOG/3.160E+00	1.89E+12	-3.00	-8995.0/
PLOG/3.160E+00	4.99E+15	-1.62	1849.0/
! fit btw. 400 and 2200 K with MAE of 1.1%, 3.2%			
PLOG/1.000E+01	1.93E+24	-5.63	1.8/
PLOG/1.000E+01	9.33E+16	-1.96	3324.0/
! fit btw. 400 and 2200 K with MAE of 1.3%, 2.9%			
PLOG/3.160E+01	1.10E+18	-2.22	5178.0/
PLOG/3.160E+01	1.02E+72	-20.69	15860.0/
! fit btw. 400 and 2200 K with MAE of 1.7%, 3.6%			
PLOG/1.000E+02	5.79E+32	-6.45	16810.0/
PLOG/1.000E+02	1.10E+09	0.31	1024.0/
! fit btw. 400 and 2200 K with MAE of 1.5%, 5.8%			

C2H3+O2=CO2+CH3 6.16E+13 -1.05
3743.0

PLOG/1.000E-02	2.37E+35	-7.76	12630.0/
PLOG/1.000E-02	6.27E+13	-1.16	406.3/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.8%			
PLOG/1.000E-01	1.73E+35	-7.72	12520.0/
PLOG/1.000E-01	6.24E+13	-1.16	401.4/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.9%			
PLOG/3.160E-01	4.47E+34	-7.55	12140.0/
PLOG/3.160E-01	6.12E+13	-1.16	397.0/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.9%			
PLOG/1.000E+00	7.25E+31	-6.70	10440.0/
PLOG/1.000E+00	5.32E+13	-1.14	446.7/
! fit btw. 400 and 2200 K with MAE of 0.3%, 0.8%			
PLOG/3.160E+00	3.63E+35	-7.75	12830.0/
PLOG/3.160E+00	1.45E+14	-1.26	987.7/
! fit btw. 400 and 2200 K with MAE of 0.2%, 0.6%			
PLOG/1.000E+01	2.09E+35	-7.53	14050.0/
PLOG/1.000E+01	5.02E+13	-1.11	1409.0/
! fit btw. 400 and 2200 K with MAE of 0.4%, 1.7%			
PLOG/3.160E+01	3.84E+18	-2.44	5408.0/
PLOG/3.160E+01	1.40E+70	-20.11	15430.0/
! fit btw. 400 and 2200 K with MAE of 1.8%, 3.8%			
PLOG/1.000E+02	1.21E+32	-6.32	16190.0/
PLOG/1.000E+02	9.21E+08	0.25	855.3/
! fit btw. 400 and 2200 K with MAE of 1.8%, 6.5%			

!CH2CHOO=CHCHO+OH 5.89E+36 -7.10
51440.0

! PLOG/1.000E-02	3.64E+49	-12.13	67420.0/
! PLOG/1.000E-02	1.17E+56	-14.81	60700.0/
! fit btw. 400 and 1250 K with MAE of 3.1%, 15.2%			
! PLOG/1.000E-01	1.44E+36	-9.92	41220.0/
! PLOG/1.000E-01	2.32E+40	-9.39	50420.0/
! fit btw. 400 and 1350 K with MAE of 4.3%, 10.0%			
! PLOG/3.160E-01	4.18E+40	-10.53	43670.0/

! PLOG/3.160E-01 1.61E+43 -9.99 50290.0/
! fit btw. 400 and 1450 K with MAE of 4.8%, 12.2%
! PLOG/1.000E+00 3.79E+46 -10.72 51900.0/
! PLOG/1.000E+00 2.33E+124 -36.77 70100.0/
! fit btw. 400 and 1550 K with MAE of 5.4%, 16.5%
! PLOG/3.160E+00 1.60E+49 -11.24 54150.0/
! PLOG/3.160E+00 1.88E+103 -29.49 65410.0/
! fit btw. 400 and 1650 K with MAE of 6.4%, 20.8%
! PLOG/1.000E+01 2.38E+51 -11.64 56980.0/
! PLOG/1.000E+01 5.96E+86 -23.81 62170.0/
! fit btw. 400 and 1750 K with MAE of 7.2%, 24.5%
! PLOG/3.160E+01 2.00E+54 -12.22 61840.0/
! PLOG/3.160E+01 1.51E+57 -13.94 55390.0/
! fit btw. 400 and 1900 K with MAE of 7.7%, 27.4%
! PLOG/1.000E+02 9.54E+195 -52.27 163500.0/
! PLOG/1.000E+02 1.79E+34 -6.40 50000.0/
! fit btw. 400 and 2100 K with MAE of 5.2%, 31.2%

CH2CHOO=CH2CHO+O 1.22E+29 -4.71
42340.0

PLOG/1.000E-02 2.70E+180 -48.19 169300.0/
PLOG/1.000E-02 1.47E+30 -6.64 41110.0/
! fit btw. 400 and 1250 K with MAE of 0.9%, 2.1%
PLOG/1.000E-01 3.90E+38 -8.69 42770.0/
PLOG/1.000E-01 9.65E-12 5.96 22890.0/
! fit btw. 400 and 1350 K with MAE of 0.6%, 1.5%
PLOG/3.160E-01 4.57E+47 -11.21 47050.0/
PLOG/3.160E-01 3.95E+22 -3.71 36270.0/
! fit btw. 400 and 1450 K with MAE of 0.9%, 1.8%
PLOG/1.000E+00 7.62E+81 -21.28 65080.0/
PLOG/1.000E+00 2.39E+33 -6.62 41280.0/
! fit btw. 400 and 1550 K with MAE of 0.6%, 1.9%
PLOG/3.160E+00 1.86E+68 -16.83 60680.0/
PLOG/3.160E+00 6.37E+31 -5.96 41260.0/
! fit btw. 400 and 1650 K with MAE of 0.6%, 2.1%
PLOG/1.000E+01 2.02E+55 -12.69 55840.0/
PLOG/1.000E+01 2.13E+29 -5.10 40710.0/
! fit btw. 400 and 1750 K with MAE of 0.7%, 2.3%
PLOG/3.160E+01 1.11E+53 -11.79 56690.0/
PLOG/3.160E+01 4.66E+27 -4.50 40530.0/
! fit btw. 400 and 1900 K with MAE of 0.9%, 3.1%
PLOG/1.000E+02 4.30E+48 -10.31 56090.0/
PLOG/1.000E+02 5.99E+25 -3.85 40120.0/
! fit btw. 400 and 2100 K with MAE of 1.2%, 3.3%

!CH2CHOO=OCHCHO+H 4.72E+20 -2.69
32320.0

! PLOG/1.000E-02 6.41E+80 -22.20 51750.0/
! PLOG/1.000E-02 1.19E+28 -6.01 28740.0/
! fit btw. 400 and 1250 K with MAE of 0.4%, 1.0%
! PLOG/1.000E-01 3.31E+65 -17.01 48090.0/
! PLOG/1.000E-01 1.40E+25 -4.80 28940.0/
! fit btw. 400 and 1350 K with MAE of 0.4%, 1.1%
! PLOG/3.160E-01 5.98E+51 -12.62 43000.0/
! PLOG/3.160E-01 2.91E+20 -3.29 27550.0/
! fit btw. 400 and 1450 K with MAE of 0.5%, 1.4%
! PLOG/1.000E+00 1.48E+44 -10.12 40790.0/

! PLOG/1.000E+00 1.58E+19 -2.82 27620.0/
! fit btw. 400 and 1550 K with MAE of 1.0%, 4.2%
! PLOG/3.160E+00 1.26E+59 -14.33 51390.0/
! PLOG/3.160E+00 1.93E+22 -3.54 29980.0/
! fit btw. 400 and 1650 K with MAE of 0.4%, 1.9%
! PLOG/1.000E+01 4.93E+26 -4.67 34320.0/
! PLOG/1.000E+01 7.51E+29 -5.75 34490.0/
! fit btw. 400 and 1750 K with MAE of 7.1%, 42.7%
! PLOG/3.160E+01 2.06E+33 -6.38 39520.0/
! PLOG/3.160E+01 7.14E+61 -16.16 43280.0/
! fit btw. 450 and 1900 K with MAE of 1.5%, 4.7%
! PLOG/1.000E+02 1.30E+32 -5.92 40660.0/
! PLOG/1.000E+02 1.14E+19 -2.56 29670.0/
! fit btw. 400 and 2100 K with MAE of 3.4%, 12.0%

CH2CHOO=CH2CO+OH 1.55E+24 -3.87
49850.0

PLOG/1.000E-02 1.15E+47 -12.28 75330.0/
PLOG/1.000E-02 2.31E+02 -0.73 25710.0/
! fit btw. 400 and 1250 K with MAE of 1.0%, 3.0%
PLOG/1.000E-01 8.43E+09 -2.06 33720.0/
PLOG/1.000E-01 1.83E-23 7.84 20190.0/
! fit btw. 400 and 1350 K with MAE of 0.2%, 0.6%
PLOG/3.160E-01 6.06E+04 0.17 34220.0/
PLOG/3.160E-01 3.82E+63 -20.44 43420.0/
! fit btw. 400 and 1450 K with MAE of 1.1%, 3.0%
PLOG/1.000E+00 1.51E+19 -3.61 43060.0/
PLOG/1.000E+00 3.18E+27 -7.76 37230.0/
! fit btw. 400 and 1550 K with MAE of 1.5%, 3.6%
PLOG/3.160E+00 2.13E+33 -7.39 51610.0/
PLOG/3.160E+00 2.32E-05 3.47 31560.0/
! fit btw. 400 and 1650 K with MAE of 1.2%, 3.2%
PLOG/1.000E+01 4.44E+36 -7.99 54680.0/
PLOG/1.000E+01 1.06E-01 2.64 34160.0/
! fit btw. 400 and 1750 K with MAE of 1.6%, 4.3%
PLOG/3.160E+01 1.19E+37 -7.80 56460.0/
PLOG/3.160E+01 5.62E+02 1.70 36450.0/
! fit btw. 400 and 1900 K with MAE of 2.1%, 6.3%
PLOG/1.000E+02 9.08E+35 -7.21 57550.0/
PLOG/1.000E+02 1.11E+07 0.52 38670.0/
! fit btw. 400 and 2100 K with MAE of 2.8%, 9.8%

! Replace HCO with 70% H + CO
! CH2CHOO=CH2O+HCO 1.19E+20 -2.29
30170.0

! PLOG/1.000E-02 5.54E+174 -55.52 60320.0/
! PLOG/1.000E-02 7.56E+35 -7.97 31280.0/
! fit btw. 400 and 1250 K with MAE of 1.5%, 4.0%
! PLOG/1.000E-01 3.01E+67 -17.25 48120.0/
! PLOG/1.000E-01 6.93E+26 -4.96 28780.0/
! fit btw. 400 and 1350 K with MAE of 0.4%, 1.1%
! PLOG/3.160E-01 6.08E+43 -9.87 37960.0/
! PLOG/3.160E-01 4.82E+20 -3.08 26630.0/
! fit btw. 400 and 1450 K with MAE of 1.0%, 1.8%
! PLOG/1.000E+00 2.88E+34 -6.88 34370.0/
! PLOG/1.000E+00 3.52E+130 -39.38 54700.0/
! fit btw. 400 and 1550 K with MAE of 1.2%, 3.2%
! PLOG/3.160E+00 2.43E+172 -43.53 191900.0/

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! PLOG/3.160E+00      7.84E+34      -6.87      35700.0/
! fit btw. 550 and 1650 K with MAE of 0.9%, 4.4%
! PLOG/1.000E+01      3.43E+32      -6.06      35500.0/
! PLOG/1.000E+01      7.27E+175     -53.78     68500.0/
! fit btw. 450 and 1750 K with MAE of 2.6%, 13.6%
! PLOG/3.160E+01      6.17E+34      -6.57      38510.0/
! PLOG/3.160E+01      3.56E+185     -54.22     88990.0/
! fit btw. 550 and 1900 K with MAE of 2.0%, 5.4%
! PLOG/1.000E+02      1.90E+30      -5.19      36800.0/
! PLOG/1.000E+02      1.56E+03       1.81      18100.0/
! fit btw. 400 and 2100 K with MAE of 4.6%, 10.6%

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CH2CHOO=CH2O+HCO                                1.19E+20      -2.29
30170.0

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PLOG/1.000E-02      1.66E+174     -55.52     60320.0/
PLOG/1.000E-02      2.27E+35      -7.97     31280.0/
! fit btw. 400 and 1250 K with MAE of 1.5%, 4.0%
PLOG/1.000E-01      9.03E+66     -17.25     48120.0/
PLOG/1.000E-01      2.08E+26      -4.96     28780.0/
! fit btw. 400 and 1350 K with MAE of 0.4%, 1.1%
PLOG/3.160E-01      1.82E+43      -9.87     37960.0/
PLOG/3.160E-01      1.45E+20      -3.08     26630.0/
! fit btw. 400 and 1450 K with MAE of 1.0%, 1.8%
PLOG/1.000E+00      8.64E+33      -6.88     34370.0/
PLOG/1.000E+00      1.06E+130     -39.38     54700.0/
! fit btw. 400 and 1550 K with MAE of 1.2%, 3.2%
PLOG/3.160E+00      7.29E+171     -43.53     191900.0/
PLOG/3.160E+00      2.35E+34      -6.87     35700.0/
! fit btw. 550 and 1650 K with MAE of 0.9%, 4.4%
PLOG/1.000E+01      1.03E+32      -6.06     35500.0/
PLOG/1.000E+01      2.18E+175     -53.78     68500.0/
! fit btw. 450 and 1750 K with MAE of 2.6%, 13.6%
PLOG/3.160E+01      1.85E+34      -6.57     38510.0/
PLOG/3.160E+01      1.07E+185     -54.22     88990.0/
! fit btw. 550 and 1900 K with MAE of 2.0%, 5.4%
PLOG/1.000E+02      5.70E+29      -5.19     36800.0/
PLOG/1.000E+02      4.68E+02       1.81     18100.0/
! fit btw. 400 and 2100 K with MAE of 4.6%, 10.6%

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CH2CHOO=CH2O+H+CO                                1.19E+20      -2.29
30170.0

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PLOG/1.000E-02      3.88E+174     -55.52     60320.0/
PLOG/1.000E-02      5.29E+35      -7.97     31280.0/
! fit btw. 400 and 1250 K with MAE of 1.5%, 4.0%
PLOG/1.000E-01      2.11E+67     -17.25     48120.0/
PLOG/1.000E-01      4.85E+26      -4.96     28780.0/
! fit btw. 400 and 1350 K with MAE of 0.4%, 1.1%
PLOG/3.160E-01      4.26E+43      -9.87     37960.0/
PLOG/3.160E-01      3.37E+20      -3.08     26630.0/
! fit btw. 400 and 1450 K with MAE of 1.0%, 1.8%
PLOG/1.000E+00      2.02E+34      -6.88     34370.0/
PLOG/1.000E+00      2.46E+130     -39.38     54700.0/
! fit btw. 400 and 1550 K with MAE of 1.2%, 3.2%
PLOG/3.160E+00      1.70E+172     -43.53     191900.0/
PLOG/3.160E+00      5.49E+34      -6.87     35700.0/
! fit btw. 550 and 1650 K with MAE of 0.9%, 4.4%
PLOG/1.000E+01      2.40E+32      -6.06     35500.0/

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PLOG/1.000E+01 5.09E+175 -53.78 68500.0/
 ! fit btw. 450 and 1750 K with MAE of 2.6%, 13.6%
 PLOG/3.160E+01 4.32E+34 -6.57 38510.0/
 PLOG/3.160E+01 2.49E+185 -54.22 88990.0/
 ! fit btw. 550 and 1900 K with MAE of 2.0%, 5.4%
 PLOG/1.000E+02 1.33E+30 -5.19 36800.0/
 PLOG/1.000E+02 1.09E+03 1.81 18100.0/
 ! fit btw. 400 and 2100 K with MAE of 4.6%, 10.6%

CH2CHOO=CO+CH3O 1.16E-01 3.16
 18420.0

PLOG/1.000E-02 5.20E+33 -7.92 31320.0/
 PLOG/1.000E-02 2.31E+129 -41.86 45850.0/
 ! fit btw. 400 and 1250 K with MAE of 1.5%, 4.1%
 PLOG/1.000E-01 1.26E+98 -27.09 64060.0/
 PLOG/1.000E-01 2.42E+28 -5.99 30540.0/
 ! fit btw. 400 and 1350 K with MAE of 0.3%, 0.9%
 PLOG/3.160E-01 1.80E+33 -7.27 33760.0/
 PLOG/3.160E-01 8.69E-50 16.63 -3900.0/
 ! fit btw. 400 and 1450 K with MAE of 1.1%, 3.6%
 PLOG/1.000E+00 3.83E+33 -7.20 35100.0/
 PLOG/1.000E+00 1.19E-39 13.61 -1317.0/
 ! fit btw. 400 and 1550 K with MAE of 0.9%, 3.5%
 PLOG/3.160E+00 1.28E+79 -19.61 74870.0/
 PLOG/3.160E+00 8.80E+86 -23.08 61010.0/
 ! fit btw. 500 and 1650 K with MAE of 19.5%, 211.3%
 PLOG/1.000E+01 4.07E+32 -6.62 37210.0/
 PLOG/1.000E+01 1.27E+03 1.44 18660.0/
 ! fit btw. 450 and 1750 K with MAE of 1.6%, 4.5%
 PLOG/3.160E+01 6.86E+44 -10.04 47030.0/
 PLOG/3.160E+01 1.97E+17 -2.23 28590.0/
 ! fit btw. 500 and 1900 K with MAE of 1.7%, 8.5%
 PLOG/1.000E+02 -1.07E+04 1.33 15620.0/
 PLOG/1.000E+02 1.16E-07 4.81 12010.0/
 ! fit btw. 400 and 2100 K with MAE of 40.4%, 163.4%

CH2CHOO=CO2+CH3 6.03E-03 3.46
 17420.0

PLOG/1.000E-02 5.09E+33 -7.95 31290.0/
 PLOG/1.000E-02 4.20E+122 -39.75 43640.0/
 ! fit btw. 400 and 1250 K with MAE of 1.5%, 4.0%
 PLOG/1.000E-01 1.21E+118 -33.13 73790.0/
 PLOG/1.000E-01 1.96E+29 -6.29 30920.0/
 ! fit btw. 400 and 1350 K with MAE of 0.4%, 1.1%
 PLOG/3.160E-01 8.56E+32 -7.21 33550.0/
 PLOG/3.160E-01 5.10E-66 21.37 -11110.0/
 ! fit btw. 400 and 1450 K with MAE of 1.2%, 3.4%
 PLOG/1.000E+00 3.27E+33 -7.22 34990.0/
 PLOG/1.000E+00 1.76E-47 15.85 -5283.0/
 ! fit btw. 400 and 1550 K with MAE of 0.9%, 3.6%
 PLOG/3.160E+00 3.49E-79 25.01 -21020.0/
 PLOG/3.160E+00 3.82E+32 -6.80 35690.0/
 ! fit btw. 550 and 1650 K with MAE of 0.9%, 3.9%
 PLOG/1.000E+01 8.16E+32 -6.76 37270.0/
 PLOG/1.000E+01 4.62E+00 2.10 17170.0/
 ! fit btw. 450 and 1750 K with MAE of 1.8%, 7.5%
 PLOG/3.160E+01 7.01E+37 -8.06 42200.0/

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PLOG/3.160E+01    3.49E+14    -1.58    26470.0/  
! fit btw. 500 and 1900 K with MAE of 2.2%, 10.5%  
PLOG/1.000E+02    -2.51E+03     1.41    14420.0/  
PLOG/1.000E+02     4.05E-09     5.14    10480.0/  
! fit btw. 400 and 2100 K with MAE of 40.7%, 150.7%
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END