```
!VERSION:  ARAMCOMECH 1.3 C4
!AUTHORS:  S. BURKE, C. ZHOU, W. K. METCALFE H. J. CURRAN
!WEBSITE: HTTP://C3.NUIGALWAY.IE/
!
!   some modifications to deal with bc5h10 as fuel
!   Each new line is noted as CW2
!
!   add Pierre's c5h9 + ho2 reaction paths
!-------------------------------------------------------------------------
-----!
ELEMENTS
C
H
N
O
AR
HE
END
!-------------------------------------------------------------------------
-----!
SPECIES
H                   H2                  O                   O2
OH                  OH*                 H2O                 N2
HO2                 H2O2                AR                  CO
CO2                 CH2O                HCO                 HO2CHO
HCOH                O2CHO               HOCHO               OCHO
HOCH2O2H            HOCH2O2             OCH2O2H             HOCH2O
CH3OH               CH2OH               CH3O                CH3O2H
CH3O2               CH4                 CH3                 CH2
CH2(S)              C                   CH                  CH*
C2H6                C2H5                C2H4                C2H3
C2H2                C2H                 CH3CHO              C2H3OH
C2H2OH              CH3CO               CH2CHO              O2CH2CHO
HO2CH2CO            CH2CO               HCCO                HCCOH
CH3CO3H             CH3CO3              CH3CO2              C2H5OH
C2H5O               PC2H4OH             SC2H4OH             O2C2H4OH
C2H5O2H             C2H5O2              C2H4O2H             C2H4O1-2
C2H3O1-2            CH3COCH3            CH3COCH2            CH3COCH2O2
C3KET21             C2H3CHO             C2H3CO              C2H5CHO
C2H5CO              CH3OCH3             CH3OCH2             CH3OCH2O2
CH2OCH2O2H          CH3OCH2O2H          CH3OCH2O            O2CH2OCH2O2H
HO2CH2OCHO          OCH2OCHO            HOCH2OCO            CH3OCHO
CH3OCO              CH2OCHO             HE                  C3H8
IC3H7               NC3H7               C3H6                C3H5-A
C3H5-S              C3H5-T              C3H4-P              C3H4-A
C3H3                C3H5O               C3H6OOH1-2          C3H6OOH1-3
C3H6OOH2-1          C3H6OOH1-2O2        C3H6OOH1-3O2        C3H6OOH2-1O2
C3H6OOH2-2          NC3H7O2H            IC3H7O2H            NC3H7O2
IC3H7O2             NC3H7O              IC3H7O              C3H6O1-2
C3H6O1-3            C3KET12             C3KET13             C3H51-2,3OOH
C3H52-1,3OOH        C3H6OH1-2           HOC3H6O2            CH3CHCO
AC3H5OOH            C2H3OOH             CC3H4               H2CC
C4H10               C4H8-1              C4H8-2              PC4H9
SC4H9               C4H71-1             C4H71-2             C4H71-3
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C4H71-4 C4H72-2 C4H6 PC4H9O2H
SC4H9O2H PC4H9O2 SC4H9O2 PC4H9O
SC4H9O C4H7O C4H8O1-2 C4H8O1-3
C4H8O1-4 C4H8O2-3 PC4H8OH SC4H8OH
C4H8OH-1O2 C4H8OH-2O2 C4H8OOH1-1 C4H8OOH1-2
C4H8OOH1-3 C4H8OOH1-4 C4H8OOH2-1 C4H8OOH2-2
C4H8OOH2-3 C4H8OOH2-4 C4H8OOH1-2O2 C4H8OOH1-3O2
C4H8OOH1-4O2 C4H8OOH2-1O2 C4H8OOH2-3O2 C4H8OOH2-4O2
NC4KET12 NC4KET13 NC4KET14 NC4KET21
NC4KET23 NC4KET24 C2H5COCH3 C2H5COCH2
CH2CH2COCH3 CH3CHCOCH3 C2H3COCH3 CH3CHOOCOCH3
CH2CHOOHCOCH3 NC3H7CHO NC3H7CO C3H6CHO-1
C3H6CHO-2 C3H6CHO-3 C2H5CHCO SC3H5CHO
SC3H5CO CH2CH2CHO IC4H10 IC4H9
TC4H9 IC4H8 IC4H7 TC4H9O2
IC3H5OCH2 IC4H7-I1 IC4H8OH1-2 TC4H8OH-I
SC4H7OH-I CCYCCC H15DE25DM H15DE25DM-S
H15DE25DM-A H15DE25DM-AO2H H15DE25DM-AO H15DE2M-T
H15DE2MCHO H15DE25DM-SO2H H15DE25DM-SO
H15DE25DM3KETO
IC4H7CHO AC5H10 AC5H9-A2 I2C4H7CHO
IC4H7O2 IC4H6OOH-I C*CYCCOC
CCYCCOOC-T1 CCYCCOOC-I2 CHOIC3H6O CCY(C2O)CO
CCYCCO-T1 C2CYCOOC-I1 IC3H5OOCH2 B2E3M1OJ
B13DE2M B1E2M4J B13DE2MJ B1E2M3J
B1E3MJ B1E2M3OJ B2E2M1OJ B1E3M3OJ
B1E3M3J B12DE3M TC4H7O2H-CYII TC3H5OOH
IC4H9O2 TC4H8O2H-I IC4H8O2H-I IC4H8O2H-T
IC4H8O CC4H8O IC4H9O TC4H9O
IC4H9O2H TC4H9O2H IC4H7O IC4H8OH
IO2C4H8OH IC3H7CHO TC3H6CHO IC3H7CO
IC3H6CHO TC4H8OOH-IO2 IC4H8OOH-IO2 IC4H8OOH-TO2
IC4KETII IC4KETIT IC4H7OH IC4H6OH
IC3H5CHO IC3H5CO TC3H6OCHO IC3H6CO
IC4H7OOH TC3H6OHCHO C3H6OH2-1 IC3H5OH
TC3H6O2CHO TC3H6O2HCO IC3H5O2HCHO CH2CCH2OH
TC4H8CHO O2C4H8CHO O2HC4H8CO C3H5OH
TIC4H7Q2-I IIC4H7Q2-T IIC4H7Q2-I CH2O2H
C4H4 C4H3-I C4H3-N C4H612
C4H2 C4H5-I C4H5-N CH3CHCHCO
CH2CHCHCHO C4H6O25 C2H3CHOCH2 C4H5-2
C4H6-2 C4H6O23 CH3CHCHCHO C4H4O
H2C4O C2H3OCH2 H2C4O C6H6
C*CCJC*C C5H6 C6H5 C6H2
C6H3 L-C6H4 C-C6H4 C6H5O
C6H5OH P-C6H4O2 O-C6H4O2 P-C6H3O2
C5H6 C5H5 C5H4O C5H5O
C5H5OH C5H4OH C5H3O C6H5OO
C6H5OOH OC6H4OH C6H4OH O-OC6H5OJ
P-OC6H5OJ C#CC*CCJ C5H6-L CJ*CC*CC*O
C*CC*CCJ*O CJ*CC*O C5H7 OC5H7O
C*CCJC*COH C*CC*CCJ C*CC*CC C*CC*CCOH
C*CCJC*O OC4H6O OC4H5O HOCO
HOC*CC*O HOC*CCJ*O O2CCHOOJ C2H3OCH2

C6H10 C6H9-A C3H2 C3H2(S)
C3H2C H2CCC(S) C3H3O C3H3O2H
C2HCHO CH3COCH2O C6H5CH3 C6H5CH2
PC3H4OH-2 SC3H4OH SC3H5OH CH3CHCHO
SC3H4OH C6H11 AC4H7OOH
NC5H12 C5H11-1 C5H11-2
C5H11-3 C5H10-1 C5H10-2 C5H81-3
C5H91-3 C5H91-4 C5H91-5 C5H92-4
C5H92-5 C5H9O1-3 C5H9O2-4 C5H11O2H-1
C5H11O2H-2 C5H11O2H-3 C5H11O2-1 C5H11O2-2
C5H11O2-3 C5H11O-1 C5H11O-2 C5H11O-3
C5H10OOH1-2 C5H10OOH1-3 C5H10OOH1-4 C5H10OOH1-5
C5H10OOH2-1 C5H10OOH2-3 C5H10OOH2-4 C5H10OOH2-5
C5H10OOH3-1 C5H10OOH3-2 C5H10O1-2 C5H10O1-3
C5H10O1-4 C5H10O1-5 C5H10O2-3 C5H10O2-4
C5H10OOH1-2O2 C5H10OOH1-3O2 C5H10OOH1-4O2 C5H10OOH1-5O2
C5H10OOH2-1O2 C5H10OOH2-3O2 C5H10OOH2-4O2 C5H10OOH2-5O2
C5H10OOH3-1O2 C5H10OOH3-2O2
C5H91-2,3OOH C5H91-2,4OOH C5H91-2,5OOH C5H91-3,4OOH
C5H91-3,5OOH C5H91-4,5OOH C5H92-1,3OOH C5H92-1,4OOH
C5H92-1,5OOH C5H92-3,4OOH C5H92-3,5OOH C5H92-4,5OOH
C5H93-1,2OOH C5H93-1,4OOH C5H93-1,5OOH C5H93-2,4OOH
C5H91-3OOH C5H91-4OOH C5H91-5OOH C5H92-1OOH
C5H92-4OOH C5H92-5OOH C5H9O1-2OOH-3 C5H9O1-2OOH-4
C5H9O1-2OOH-5 C5H9O1-3OOH-2 C5H9O1-3OOH-4 C5H9O1-3OOH-5
C5H9O1-4OOH-2 C5H9O1-4OOH-3 C5H9O1-4OOH-5 C5H9O1-5OOH-2
C5H9O1-5OOH-3 C5H9O2-3OOH-1 C5H9O2-3OOH-4 C5H9O2-3OOH-5
C5H9O2-4OOH-1 C5H9O2-4OOH-3 OCH2CHO C5H9O1-2O-5
CH2OCH2CHO C2H4OCHO CH2CH2OCH2CH2CHO C4H7O1-4
NC5KET12 NC5KET13 NC5KET14 NC5KET15
NC5KET21 NC5KET23 NC5KET24 NC5KET25
NC5KET31 NC5KET32 CHOC4H8O
CHOCH2CH2C2H4O
CHOCH2CH2CH2CH2O C3H7COCH2O CH3COC3H6O
CH3COCH2CH2CH2O
C2H5COC2H4O CH3COCH2C2H4O CHOCH2C3H6O C2H5COCH2CH2O
C5H10OH-1 C5H10OH-2 O2C5H10OH-1 O2C5H10OH-2
IC5H12 AC5H11 BC5H11 CC5H11
DC5H11 AC5H10 BC5H10 CC5H10
AC5H9-C AC5H9-D CC5H9-A
CC5H9-B AC5H9O-A2 AC5H9O-C CC5H9O-B
BC5H9O-A BC5H9O-D
AC5H11O2H BC5H11O2H CC5H11O2H DC5H11O2H
AC5H11O2 BC5H11O2 CC5H11O2 DC5H11O2
AC5H11O BC5H11O CC5H11O DC5H11O
AC5H10OOH-A AC5H10OOH-B AC5H10OOH-C AC5H10OOH-D
BC5H10OOH-A BC5H10OOH-C BC5H10OOH-D CC5H10OOH-A
CC5H10OOH-B CC5H10OOH-D DC5H10OOH-A DC5H10OOH-B
DC5H10OOH-C A-AC5H10O A-BC5H10O A-CC5H10O
A-DC5H10O B-CC5H10O B-DC5H10O C-DC5H10O
AC5H10OOH-AO2 AC5H10OOH-BO2 AC5H10OOH-CO2 AC5H10OOH-DO2
BC5H10OOH-AO2 BC5H10OOH-CO2 BC5H10OOH-DO2 CC5H10OOH-AO2
CC5H10OOH-BO2 CC5H10OOH-DO2 DC5H10OOH-AO2 DC5H10OOH-BO2
DC5H10OOH-CO2 C5H9A-A,BOOH

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C5H9A-A,COOH        C5H9A-A,DOOH        C5H9A-B,COOH        C5H9A-B,DOOH
C5H9A-C,DOOH        C5H9B-A,AOOH        C5H9B-A,COOH        C5H9B-A,DOOH
C5H9B-C,DOOH        C5H9C-A,AOOH        C5H9C-A,BOOH        C5H9C-A,DOOH
C5H9C-B,DOOH        C5H9D-A,AOOH        C5H9D-A,BOOH        C5H9D-A,COOH
C5H9D-B,COOH        C5H9A-AOOH          C5H9A-COOH          C5H9A-DOOH
C5H9B-AOOH          C5H9B-DOOH          C5H9C-AOOH          C5H9C-BOOH
C5H9OA-AOOH-B       C5H9OA-AOOH-C       C5H9OA-AOOH-D
C5H9OA-BOOH-A       C5H9OA-BOOH-C       C5H9OA-BOOH-D       C5H9OA-COOH-A
C5H9OA-COOH-B       C5H9OA-COOH-D       C5H9OA-DOOH-A       C5H9OA-DOOH-B
C5H9OA-DOOH-C       C5H9OB-COOH-A       C5H9OB-COOH-D       C5H9OB-DOOH-A
C5H9OB-DOOH-C       C5H9OC-DOOH-A       C5H9OC-DOOH-B       C4H7O2-1
CC3H5OCH2           CH3COCH2OCH2CH2     IC5KETAA            IC5KETAB
IC5KETAC            IC5KETAD            IC5KETCA            IC5KETCB
IC5KETCD            IC5KETDA            IC5KETDB            IC5KETDC
C2H5CH(CH2O)CHO     C3H5O(CH3)CHO       C2H4OCH(CH3)CHO     CH2OC3H6CHO
CH3COCH(CH3)CH2O    CH3CO(CH3)C2H3O     CH2OCOCH(CH3)CH3    CHOC3H6CH2O
CHOCH2(CH3)C2H3O    CHOCHOCH(CH3)CH3    AC5H10OH            BC5H10OH
CC5H10OH            AO2C5H10OH          BO2C5H10OH          CO2C5H10OH
IC3H5COCH3          IC3H5COCH2          AC3H4COCH3          NEOC5H12
NEOC5H11            NEOC5H11O2H         NEOC5H11O2          NEOC5H11O
NEOC5H10OOH         NEO-C5H10O          NEOC5H10OOH-O2      NEOC5H9Q2
NEOC5KET            NEOC5KETOX          NEOC5KEJOL
IC4H6Q2-II          NEOC5H9O-OOH        HO2CH2CHO           C4H71-3OOH
C4H71-4OOH          C4H72-1OOH
IC5H8
END
!------------------------------------------------------------------------
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REACTIONS

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

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

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

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

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

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

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

!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                                 3.000E+013     0.000
0.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
HCO+HCO=>H2+CO+CO                                 3.000E+012     0.000
0.0

!REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987)
HCO+CH3<=>CH4+CO                                  2.650E+013     0.000
0.0

!REF:N. K. SRINIVASAN ET AL.,J. PHYS. CHEM. A 109, 7902-7914 (2005)
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CH2O+O2<=>HCO+HO2                                   8.070E+015     0.000
53420.0

!REF:
HCO+O2<=>O2CHO                                      1.200E+011     0.000
-1100.0

!REF:ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986
CH2O+O2CHO<=>HCO+HO2CHO                             1.990E+012     0.000
11660.0

!REF:WKM ESTIMATE
OCHO+OH<=>HO2CHO                                    2.000E+013     0.000
0.0

!REF:
H+CO2<=>OCHO                                        7.500E+013     0.000
29000.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
HCO+HCO<=>CH2O+CO                                   1.800E+013     0.000
0.0

!REF:OH* KATHROTIA ET AL. COMB & FLAME 2010
H+O+M<=>M+OH*                                       1.500E+013     0.000
5975.0
H2/ 1.00/ H2O/ 6.50/ O2/ 0.40/ N2/ 0.40/ AR/ 0.35/
OH*+H2O<=>OH+H2O                                    5.930E+012     0.500
-860.0
OH*+H2<=>OH+H2                                      2.950E+012     0.500
-444.0
OH*+N2<=>OH+N2                                      1.080E+011     0.500
-1242.0
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
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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
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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                                  4.240E+006     2.100
4868.0

!REF:MARINOV ESTIMATE
HOCHO+H=>H2+CO+OH                                  6.030E+013    -0.350
2988.0
HOCHO+CH3=>CH4+CO+OH                               3.900E-007     5.800
2200.0

!REF: CURRAN ESTIMATE
OCHO+H2O2<=>HOCHO+HO2                              2.400E+012     0.000
10000.0

!REF:MARINOV ESTIMATE
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HOCHO+HO2=>H2O2+CO+OH                                1.000E+012     0.000
11920.0

!REF:MARINOV ESTIMATE
HOCHO+O=>CO+OH+OH                                    1.770E+018    -1.900
2975.0

!REF:CURRAN ESTIMATE
CH2O+OCHO<=>HOCHO+HCO                                5.600E+012     0.000
13600.0

!REF:HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).
CH3O(+M)<=>CH2O+H(+M)                                6.800E+013     0.000
26170.0
LOW/                                                 1.867E+025    -3.000
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/

!REF:WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653 (1987)
CH3O+O2<=>CH2O+HO2                                   4.380E-019     9.500
-5501.0

!REF:FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998).
CH2O+CH3O<=>CH3OH+HCO                                6.620E+011     0.000
2294.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
CH3+CH3OH<=>CH4+CH3O                                 1.440E+001     3.100
6935.0

!REF:
CH3O+CH3<=>CH2O+CH4                                  1.200E+013     0.000
0.0

!REF:HOYERMANN ET AL., 18TH SYMPOSIUM
CH3O+H<=>CH2O+H2                                     2.000E+013     0.000
0.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
CH3O+HO2<=>CH2O+H2O2                                 3.010E+011     0.000
0.0

!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:GROTHEER, H. H. ET AL., J. PHYS. CHEM. 92: 4028 (1988).
CH2OH+O2<=>CH2O+HO2                                  1.510E+015    -1.000
0.0
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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/                                                1.500E+043    -6.995
97992.2/
TROE/ -4.748E-001  3.558E+004  1.116E+003  9.023E+003/
CH3OH(+M)<=>CH2(S)+H2O(+M)                          3.121E+018    -1.017
91712.0
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LOW/                                                1.430E+047    -8.227
99417.1/
TROE/  2.545E+000  3.290E+003  4.732E+004  4.711E+004/
CH3OH(+M)<=>CH2OH+H(+M)                             7.896E-003     5.038
84467.4
LOW/                                                3.390E+042    -7.244
105230.3/
TROE/ -7.391E+001  3.705E+004  4.150E+004  5.220E+003/

!REF:J. CHEM. PHYS. 134, 094302 (2011)
CH3OH+H<=>CH2OH+H2                                  3.070E+005     2.550
5440.0
CH3OH+H<=>CH3O+H2                                   1.990E+005     2.560
10300.0

!REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH3OH+O<=>CH2OH+OH                                  3.880E+005     2.500
3080.0

!REF:XU ET AL. PROC 31 2007 159-166
CH3OH+OH<=>CH2OH+H2O                                3.080E+004     2.650
-806.7
CH3OH+OH<=>CH3O+H2O                                 1.500E+002     3.030
-763.0

!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY,
1975
CH3OH+O2<=>CH2OH+HO2                                2.050E+013     0.000
44900.0

!REF:CURRAN ESTIMATE
CH3OH+HO2<=>CH2OH+H2O2                              1.080E+004     2.550
10530.0

!REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH3OH+CH3<=>CH2OH+CH4                               3.190E+001     3.170
7172.0
CH3O+CH3OH<=>CH2OH+CH3OH                            3.000E+011     0.000
4074.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
CH3O+CH3O<=>CH3OH+CH2O                              6.030E+013     0.000
0.0

!REF:GRI
CH3+H(+M)<=>CH4(+M)                                 1.270E+016    -0.630
383.0
LOW/                                                2.477E+033    -4.760
2440.0/
TROE/  7.830E-001  7.400E+001  2.941E+003  6.964E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/

!REF:BAULCH, D.L.; ET AL.,J. PHYS. CHEM. REF. DATA (2005)
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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/
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!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
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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
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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)
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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
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!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/
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PLOG/    100.0000     1.032E+002     3.230     11236.1/

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

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

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

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

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

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

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

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

!REF:BASED ON CH4+CH3O2
CH4+C2H5O2<=>CH3+C2H5O2H                            1.810E+011     0.000
18480.0

!REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH3OH+C2H5O2<=>CH2OH+C2H5O2H                        1.810E+012     0.000
13710.0
C2H5O2+HO2<=>C2H5O2H+O2                             1.750E+010     0.000
-3275.0

!REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003
C2H6+C2H5O2<=>C2H5+C2H5O2H                          8.600E+000     3.760
17200.0
C2H5O2H<=>C2H5O+OH                                  6.310E+014     0.000
42300.0
C2H5+O2<=>C2H5O2                                    3.398E+053   -13.900
9279.0
PLOG/      0.0400     3.398E+053   -13.900      9279.0/
PLOG/      1.0000     9.362E+059   -15.280     14240.0/
PLOG/     10.0000     1.262E+060   -14.910     16240.0/
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C2H5+O2<=>C2H4O2H                                   2.103E+034    -9.010
5444.0
PLOG/      0.0400     2.103E+034    -9.010      5444.0/
PLOG/      1.0000     4.884E+033    -8.310      7710.0/
PLOG/     10.0000     1.705E+045   -11.490     14590.0/
C2H5+O2<=>C2H4+HO2                                  2.094E+009     0.490
-391.4
DUP
PLOG/      0.0400     2.094E+009     0.490      -391.4/
PLOG/      1.0000     1.843E+007     1.130      -720.6/
PLOG/     10.0000     7.561E+014    -1.010      4749.0/
C2H5+O2<=>C2H4+HO2                                  6.609E+000     3.510
14160.0
DUP
C2H5+O2<=>C2H4O1-2+OH                               1.303E+003     1.930
-502.7
PLOG/      0.0400     1.303E+003     1.930      -502.7/
PLOG/      1.0000     2.438E+002     2.180       -62.5/
PLOG/     10.0000     4.621E+009     0.150      5409.0/
C2H5+O2<=>CH3CHO+OH                                 4.908E-006     4.760
254.3
PLOG/      0.0400     4.908E-006     4.760       254.3/
PLOG/      1.0000     6.803E-002     3.570      2643.0/
PLOG/     10.0000     8.265E+002     2.410      5285.0/
C2H4O2H<=>C2H5O2                                    2.653E-016     6.960
2396.0
PLOG/      0.0400     2.653E-016     6.960      2396.0/
PLOG/      1.0000     1.064E+041   -10.100     26030.0/
PLOG/     10.0000     1.203E+036    -8.130     27020.0/
C2H5O2<=>CH3CHO+OH                                  1.237E+035    -9.420
36360.0
PLOG/      0.0400     1.237E+035    -9.420     36360.0/
PLOG/      1.0000     1.687E+036    -9.220     38700.0/
PLOG/     10.0000     2.520E+041   -10.200     43710.0/
C2H5O2<=>C2H4+HO2                                   1.782E+032    -7.100
32840.0
PLOG/      0.0400     1.782E+032    -7.100     32840.0/
PLOG/      1.0000     2.701E+037    -8.470     35840.0/
PLOG/     10.0000     1.980E+038    -8.460     37900.0/
C2H5O2<=>C2H4O1-2+OH                                5.778E+045   -11.900
4112.0
PLOG/      0.0400     5.778E+045   -11.900      4112.0/
PLOG/      1.0000     1.916E+043   -10.750     42400.0/
PLOG/     10.0000     3.965E+043   -10.460     45580.0/
C2H4O2H<=>C2H4O1-2+OH                               8.959E+038    -9.400
20660.0
PLOG/      0.0400     8.959E+038    -9.400     20660.0/
PLOG/      1.0000     1.224E+037    -8.320     21460.0/
PLOG/     10.0000     8.848E+030    -6.080     20660.0/
C2H4O2H<=>C2H4+HO2                                  3.918E+040   -10.200
22250.0
PLOG/      0.0400     3.918E+040   -10.200     22250.0/
PLOG/      1.0000     6.825E+040    -9.610     23840.0/
PLOG/     10.0000     3.980E+034    -7.250     23250.0/
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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
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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: GUPTE 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/                                                5.650E+018    -0.970
14600.0/
TROE/  6.290E-001  8.730E+009  5.520E+000  7.600E+007/

!REF:
CH3CO+H<=>CH2CO+H2                                  2.000E+013     0.000
0.0
CH3CO+O<=>CH2CO+OH                                  2.000E+013     0.000
0.0
CH3CO+CH3<=>CH2CO+CH4                               5.000E+013     0.000
0.0

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

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

!REF:ANALOGY TO CH3O2+CH2O
CH2O+CH3CO3<=>HCO+CH3CO3H                              1.990E+012     0.000
11660.0

!REF: ANALOGY TO C2H6+HO2
C2H6+CH3CO3<=>C2H5+CH3CO3H                             1.700E+013     0.000
20460.0

!REF:SAHETCHIAN ET AL. 1992
CH3CO3H<=>CH3CO2+OH                                    5.010E+014     0.000
40150.0

!REF:ANALOGY TO CH3CO<=>CH3+CO
CH3CO2+M<=>CH3+CO2+M                                   4.400E+015     0.000
10500.0

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
CH2CHO(+M)<=>CH2CO+H(+M)                               1.430E+015    -0.150
45600.0

!REF:LPL TIMES 2
LOW/                                                   6.000E+029    -3.800
43423.9/
TROE/  9.850E-001  3.930E+002  9.800E+009  5.000E+009/

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
CH2CHO(+M)<=>CH3+CO(+M)                                2.930E+012     0.290
40300.0
LOW/                                                   9.520E+033    -5.070
41300.0/
TROE/  7.130E-017  1.150E+003  4.990E+009  1.790E+009/

!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/
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PLOG/     10.0000     7.050E+007     1.630     25290.0/
CH2CHO+O2=>CH2O+CO+OH                                  2.680E+017    -1.840
6530.0
PLOG/      0.0100     2.680E+017    -1.840      6530.0/
PLOG/      0.1000     1.520E+020    -2.580      8980.0/
PLOG/      1.0000     1.650E+019    -2.220     10340.0/
PLOG/     10.0000     8.953E+013    -0.600     10120.0/
CH2CHO+O2<=>HO2CH2CO                                   3.640E+065   -21.870
19020.0
PLOG/      0.0100     3.640E+065   -21.870     19020.0/
PLOG/      0.1000     3.640E+058   -19.000     19090.0/
PLOG/      1.0000     6.650E+048   -15.550     17460.0/
PLOG/     10.0000     4.800E+038   -12.140     14960.0/
O2CH2CHO<=>HO2CH2CO                                    8.270E+030    -6.650
24500.0
PLOG/      0.0100     8.270E+030    -6.650     24500.0/
PLOG/      0.1000     1.730E+026    -4.990     23760.0/
PLOG/      1.0000     9.030E+019    -2.920     22170.0/
PLOG/     10.0000     1.430E+016    -1.670     21210.0/
O2CH2CHO<=>CH2CO+HO2                                   2.050E+040   -13.310
52150.0
PLOG/      0.0100     2.050E+040   -13.310     52150.0/
PLOG/      0.1000     5.720E+045   -14.000     52200.0/
PLOG/      1.0000     4.160E+055   -15.760     55080.0/
PLOG/     10.0000     1.120E+061   -16.040     60010.0/
HO2CH2CO=>CO+CH2O+OH                                   2.360E+017    -2.950
8100.0
PLOG/      0.0100     2.360E+017    -2.950      8100.0/
PLOG/      0.1000     2.380E+018    -2.950      8100.0/
PLOG/      1.0000     2.510E+019    -2.950      8110.0/
PLOG/     10.0000     4.160E+020    -3.020      8240.0/
HO2CH2CO<=>CH2CO+HO2                                   1.120E+007    -3.760
21680.0
PLOG/      0.0100     1.120E+007    -3.760     21680.0/
PLOG/      0.1000     1.100E+008    -3.760     21680.0/
PLOG/      1.0000     9.200E+008    -3.730     21630.0/
PLOG/     10.0000     2.090E+009    -3.550     21220.0/

!REF:LASKIN ET AL. IJCK 32 589-614 2000
CH2+CO(+M)<=>CH2CO(+M)                                 8.100E+011     0.000
0.0
LOW/                                                   2.690E+033    -5.110
7095.0/
TROE/  5.907E-001  2.750E+002  1.226E+003  5.185E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/

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

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

!REF:IMPORTANT FOR ACETONE FLAME SPEEDS
CH3CO(+M)<=>CH2CO+H(+M)                                9.413E+007     1.917
44987.2
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LOW/                                                1.516E+051   -10.270
55390.0/
TROE/  6.009E-001  8.103E+009  6.677E+002  5.000E+009/

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

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

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

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

!REF:WKM CALCULATION, CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
CH2CO+CH3<=>C2H5+CO                                 4.769E+004     2.312
9468.0
CH2(S)+CH2CO<=>C2H4+CO                              1.600E+014     0.000
0.0
HCCO+OH=>H2+CO+CO                                   1.000E+014     0.000
0.0
HCCO+O=>H+CO+CO                                     8.000E+013     0.000
0.0

!REF:GRI
HCCO+H<=>CH2(S)+CO                                  1.000E+014     0.000
0.0

!REF:KLIPPENSTEIN 2002
HCCO+O2=>OH+CO+CO                                   1.910E+011    -0.020
1020.0
HCCO+O2=>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<=>HCCO+M                                    7.570E+022    -1.900
0.0

!REF:REG 2.11
CH+CH2O<=>H+CH2CO                                   9.460E+013     0.000
-515.0
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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
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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
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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
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!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

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

!REF:TO COMBAT OVER-PRODUCTION OF C2H2 IN ETHYLENE JSR
C2H3+O2<=>CH2O+HCO                                      1.700E+029    -5.312
6503.1
C2H3+O2<=>CH2CHO+O                                      7.000E+014    -0.611
5262.4
C2H3+O2=>H+CO+CH2O                                      5.190E+015    -1.260
3312.6

!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
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C2H+O2<=>HCO+CO                                          5.000E+013     0.000
1500.0
C2H+H2<=>H+C2H2                                          4.900E+005     2.500
560.0

!REF:99 LAS/ WAN
C2H2(+M)<=>H2CC(+M)                                      8.000E+014    -0.520
50750.0
LOW/                                                     2.450E+015    -0.640
49700.0/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/
2.50/ C2H4/ 2.50/

!REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
C2H2+O<=>CH2+CO                                          7.395E+008     1.280
2472.0
C2H2+O<=>HCCO+H                                          2.958E+009     1.280
2472.0
C2H2+HO2<=>CH2CO+OH                                      6.030E+009     0.000
7949.0

!REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055
C2H2+OH<=>C2H+H2O                                        2.632E+006     2.140
17060.0
C2H2+OH<=>HCCOH+H                                        2.800E+005     2.280
12420.0
PLOG/      0.0100     2.800E+005     2.280     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/
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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
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C2H5OH+H<=>SC2H4OH+H2                             8.790E+004     2.680
2910.0
C2H5OH+H<=>PC2H4OH+H2                             5.310E+004     2.810
7490.0
C2H5OH+H<=>C2H5O+H2                               9.450E+002     3.140
8701.1

!REF: SMB 04/ 09/ 2013

!REF: BRANCHING RATIO CHANGED FOR THE UNDERPREDICIOTN OF C2H4 IN THE JSR
AND FLOW REACTOR
C2H5OH+OH<=>SC2H4OH+H2O                           7.520E+004     2.490
-1474.1
C2H5OH+OH<=>PC2H4OH+H2O                           3.760E+003     2.780
-1810.2
C2H5OH+OH<=>C2H5O+H2O                             5.810E-003     4.280
-3560.0

!REF:ESTIMATED FROM CW ZHOU BUTANOL+OH

!REF: MITTAL 2013 ( INCREASED BY 1.75 ZHOU )
C2H5OH+HO2<=>SC2H4OH+H2O2                         2.450E-005     5.260
7475.1
C2H5OH+HO2<=>PC2H4OH+H2O2                         3.986E-002     4.300
15333.0
C2H5OH+HO2<=>C2H5O+H2O2                           6.470E-007     5.300
10533.1

!REF:ANAOLGY WITH C2H5OH+HO2
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H                     1.225E-005     5.260
7475.1
C2H5OH+CH3O2<=>PC2H4OH+CH3O2H                     1.995E-002     4.300
15333.0
C2H5OH+CH3O2<=>C2H5O+CH3O2H                       3.236E-007     5.300
10533.1

!REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703
C2H5OH+O<=>PC2H4OH+OH                             9.690E+002     3.230
4658.0
C2H5OH+O<=>SC2H4OH+OH                             1.450E+005     2.470
876.0
C2H5OH+O<=>C2H5O+OH                               1.460E-003     4.730
1727.0

!REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004
C2H5OH+CH3<=>PC2H4OH+CH4                          3.300E+002     3.300
12290.0
C2H5OH+CH3<=>SC2H4OH+CH4                          1.993E+001     3.370
7634.0
C2H5OH+CH3<=>C2H5O+CH4                            2.035E+000     3.570
7721.0

!REF:1/ 2 OF C4H10+C2H5
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C2H5OH+C2H5<=>PC2H4OH+C2H6                          5.000E+010     0.000
13400.0

!REF:ESTIMATE
C2H5OH+C2H5<=>SC2H4OH+C2H6                          5.000E+010     0.000
10400.0

!REF:CURRAN, FIT TO NIST DATABASE

!REF:WKM CALCULATION.
SC2H4OH<=>CH3CHO+H                                  5.690E+052   -13.380
45049.0
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                                  5.400E+046   -11.630
44323.0
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
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!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                            1.250E+005     2.483
445.0

!REF:CURRAN ESTIMATE
CH3COCH3+H<=>CH3COCH2+H2                              9.800E+005     2.430
5160.0

!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98
CH3COCH3+O<=>CH3COCH2+OH                              5.130E+011     0.211
4890.0

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

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

!REF:A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN
CH3COCH3+O2<=>CH3COCH2+HO2                            6.030E+013     0.000
48500.0
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!REF:ANALOGY TO ETHANE
CH3COCH3+HO2<=>CH3COCH2+H2O2                          1.700E+013     0.000
20460.0
CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H                      1.700E+013     0.000
20460.0

!REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
CH2CO+CH3<=>CH3COCH2                                  1.760E+004     2.480
6130.0
CH3COCH2+HO2<=>CH3COCH2O+OH                           2.410E+013     0.000
0.0
CH3COCH2+CH3O2<=>CH3COCH2O+CH3O                       1.205E+013     0.000
0.0
CH3COCH2+H<=>CH3COCH3                                 1.000E+013     0.000
0.0
CH3COCH2O<=>CH3CO+CH2O                                5.000E+010     0.000
5108.0

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

!REF:WESTBROOK ESTIMATE
CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21                1.000E+011     0.000
5000.0
CH2O+CH3COCH2O2<=>HCO+C3KET21                         1.288E+011     0.000
9000.0
HO2+CH3COCH2O2<=>C3KET21+O2                           1.000E+012     0.000
0.0

!REF:ESTIMATE
C2H3+HCO<=>C2H3CHO                                    1.810E+013     0.000
0.0

!REF:BASED ON CH3CHO+H
C2H3CHO+H<=>C2H3CO+H2                                 1.340E+013     0.000
3300.0
C2H3CHO+O<=>C2H3CO+OH                                 5.940E+012     0.000
1868.0

!REF:TAYLOR ET AL. 1996
C2H3CHO+OH<=>C2H3CO+H2O                               9.240E+006     1.500
-962.0
C2H3CHO+O2<=>C2H3CO+HO2                               1.005E+013     0.000
40700.0

!REF:BASED ON CH3CHO+HO2
C2H3CHO+HO2<=>C2H3CO+H2O2                             3.010E+012     0.000
11920.0
C2H3CHO+CH3<=>C2H3CO+CH4                              2.608E+006     1.780
5911.0

!REF:ANALOGY WITH ACETALDEHYDE.
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C2H3CHO+C2H3<=>C2H3CO+C2H4                          1.740E+012     0.000
8440.0

!REF:ANALOGY WITH CH3CHO+CH3O
C2H3CHO+CH3O<=>C2H3CO+CH3OH                         1.000E+012     0.000
3300.0

!REF:BASED ON CH3CHO+HO2
C2H3CHO+CH3O2<=>C2H3CO+CH3O2H                       3.010E+012     0.000
11920.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
C2H3+CO<=>C2H3CO                                    1.510E+011     0.000
4810.0

!REF:
C2H5+HCO<=>C2H5CHO                                  1.810E+013     0.000
0.0

!REF:ANALOGY WITH CH3CHO+H
C2H5CHO+H<=>C2H5CO+H2                               4.000E+013     0.000
4200.0

!REF:ANALOGY WITH CH3CHO+O
C2H5CHO+O<=>C2H5CO+OH                               5.000E+012     0.000
1790.0

!REF:ESTIMATE
C2H5CHO+OH<=>C2H5CO+H2O                             2.690E+010     0.760
-340.0

!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98
C2H5CHO+CH3<=>C2H5CO+CH4                            2.608E+006     1.780
5911.0

!REF:ANALOGY WITH CH3CHO+HO2
C2H5CHO+HO2<=>C2H5CO+H2O2                           2.800E+012     0.000
13600.0

!REF:!ANALOGY WITH CH3CHO+CH3O
C2H5CHO+CH3O<=>C2H5CO+CH3OH                         1.000E+012     0.000
3300.0

!REF:ANALOGY WITH CH3CHO+HO2
C2H5CHO+CH3O2<=>C2H5CO+CH3O2H                       3.010E+012     0.000
11920.0

!REF:ACETALDEHYDE ANALOG
C2H5CHO+C2H5<=>C2H5CO+C2H6                          1.000E+012     0.000
8000.0
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH                       6.026E+011     0.000
3300.0

!REF:BASED ON CH3CHO+HO2
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C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H                    3.010E+012     0.000
11920.0

!REF:ESTIMATE
C2H5CHO+O2<=>C2H5CO+HO2                            1.005E+013     0.000
40700.0

!REF:BASED ON CH3CHO+HO2
C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H                    3.010E+012     0.000
11920.0

!REF:!ANALOGY WITH ACETALDEHYDE
C2H5CHO+C2H3<=>C2H5CO+C2H4                         1.700E+012     0.000
8440.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
C2H5+CO<=>C2H5CO                                   1.510E+011     0.000
4810.0

!REF:COOK ET AL. J. PHYS. CHEM A 2009, 113, 9974-9980
CH3OCH3(+M)<=>CH3+CH3O(+M)                         4.380E+021    -1.570
83890.0
LOW/                                               7.520E+015     0.000
42790.0/
TROE/  4.540E-001  1.000E-030  2.510E+003/

!REF:ARIF M, ET AL., J. PHYS. CHEM. A, 101, 13, 2436-2441 (1997).
CH3OCH3+OH<=>CH3OCH2+H2O                           6.324E+006     2.000
-651.7

!REF:CURRAN, FIT TO NIST DATABASE
CH3OCH3+H<=>CH3OCH2+H2                             7.721E+006     2.090
3384.0

!REF:CURRAN 08 NIST FIT
CH3OCH3+O<=>CH3OCH2+OH                             7.750E+008     1.360
2250.0

!REF: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                         8.670E+002     3.010
12090.0
CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H                     3.120E+002     3.120
13190.0

!REF:
CH3OCH3+CH3<=>CH3OCH2+CH4                          1.445E-006     5.730
5700.0
CH3OCH3+O2<=>CH3OCH2+HO2                           4.100E+013     0.000
44910.0
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!REF:ESTIMATE
CH3OCH3+CH3O<=>CH3OCH2+CH3OH                          6.020E+011     0.000
4074.0

!REF:
CH3OCH3+CH3OCH2O2<=>CH3OCH2+CH3OCH2O2H                5.000E+012     0.000
17690.0
CH3OCH3+O2CHO<=>CH3OCH2+HO2CHO                        4.425E+004     2.600
13910.0
CH3OCH3+OCHO<=>CH3OCH2+HOCHO                          1.000E+013     0.000
17690.0
CH3OCH2<=>CH2O+CH3                                    1.600E+013     0.000
25500.0

!REF:ESTIMATE
CH3OCH2+CH3O<=>CH3OCH3+CH2O                           2.410E+013     0.000
0.0
CH3OCH2+CH2O<=>CH3OCH3+HCO                            5.490E+003     2.800
5862.0
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO                        1.260E+012     0.000
8499.0
CH3OCH2+O2<=>CH3OCH2O2                                2.000E+012     0.000
0.0

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

!REF:!1/ 2 CH3O2+CH2O<=>CH3O2H+HCO
CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO                       1.000E+012     0.000
11660.0

!REF:ESTIMATE
CH3OCH2O2+CH3CHO<=>CH3OCH2O2H+CH3CO                   2.800E+012     0.000
13600.0
CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O             1.547E+023    -4.500
0.0
CH3OCH2O+OH<=>CH3OCH2O2H                              2.000E+013     0.000
0.0
CH3O+CH2O<=>CH3OCH2O                                  1.000E+011     0.000
7960.0
CH3OCH2O+O2<=>CH3OCHO+HO2                             5.000E+010     0.000
500.0

!REF:
CH3OCHO+H<=>CH3OCH2O                                  1.000E+013     0.000
7838.0

!REF:ESTIMATE EA EQUALS DELTAH+RS+EABS
CH3OCH2O2<=>CH2OCH2O2H                                6.000E+010     0.000
21580.0

!REF: ESTIMATE EA<=>DELTAU+EADDN.
CH2OCH2O2H=>OH+CH2O+CH2O                              1.500E+013     0.000
20760.0
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!REF:ESTIMATE
CH2OCH2O2H+O2<=>O2CH2OCH2O2H                          7.000E+011     0.000
0.0
O2CH2OCH2O2H<=>HO2CH2OCHO+OH                          4.000E+010     0.000
18580.0
HO2CH2OCHO<=>OCH2OCHO+OH                              2.000E+016     0.000
40500.0

!REF:WKM RECOMMENDATION 8/ 9/ 2010

!REF:ESTIMATE
CH2O+OCHO<=>OCH2OCHO                                  1.250E+011     0.000
11900.0
OCH2OCHO<=>HOCH2OCO                                   1.000E+011     0.000
14000.0
HOCH2O+CO<=>HOCH2OCO                                  1.500E+011     0.000
4800.0
CH2OH+CO2<=>HOCH2OCO                                  1.500E+011     0.000
35720.0

!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.
CH2OCHO+H<=>CH3OCHO                                   1.000E+014     0.000
0.0
CH3OCO+H<=>CH3OCHO                                    1.000E+014     0.000
0.0

!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.
CH3O+HCO<=>CH3OCHO                                    3.000E+013     0.000
0.0

!REF:ESTIMATE
CH3+OCHO<=>CH3OCHO                                    1.000E+013     0.000
0.0
CH3OCHO+O2<=>CH3OCO+HO2                               1.000E+013     0.000
49700.0
CH3OCHO+O2<=>CH2OCHO+HO2                              2.050E+013     0.000
52000.0

!REF:ANOLOGY TO PROPANE
CH3OCHO+OH<=>CH3OCO+H2O                               1.580E+007     1.800
934.0
CH3OCHO+OH<=>CH2OCHO+H2O                              5.270E+009     0.970
1586.0

!REF:CURRAN ESTIMATE TSANG '88 PRIMARY H
CH3OCHO+HO2<=>CH3OCO+H2O2                             4.820E+003     2.600
13910.0

!REF:CURRAN ESTIMATE TSANG '88 SECONDARY H
CH3OCHO+HO2<=>CH2OCHO+H2O2                            2.380E+004     2.550
16490.0

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
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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:ANOLOGY 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
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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.
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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                              6.400E+004     2.170
7520.0

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
CH3+C3H8<=>CH4+NC3H7                              9.040E-001     3.650
7154.0

!REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L.,

!REF:AND GLASSMAN, I., TO BE PUBLISHED.
IC3H7+C3H8<=>NC3H7+C3H8                           3.000E+010     0.000
12900.0
C2H3+C3H8<=>C2H4+IC3H7                            1.000E+011     0.000
10400.0
C2H3+C3H8<=>C2H4+NC3H7                            1.000E+011     0.000
10400.0
C2H5+C3H8<=>C2H6+IC3H7                            1.000E+011     0.000
10400.0
C2H5+C3H8<=>C2H6+NC3H7                            1.000E+011     0.000
10400.0

!REF:DAGAUT ET AL., CST 71, 111(1990)
C3H8+C3H5-A<=>NC3H7+C3H6                          7.940E+011     0.000
20500.0
C3H8+C3H5-A<=>IC3H7+C3H6                          7.940E+011     0.000
16200.0

!REF:DRYER ESTIMATE
C3H8+CH3O<=>NC3H7+CH3OH                           3.000E+011     0.000
7000.0
C3H8+CH3O<=>IC3H7+CH3OH                           3.000E+011     0.000
7000.0

!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                         1.386E+000     3.970
18280.0
CH3O2+C3H8<=>CH3O2H+IC3H7                         1.019E+001     3.580
14810.0
C2H5O2+C3H8<=>C2H5O2H+NC3H7                       1.386E+000     3.970
18280.0
C2H5O2+C3H8<=>C2H5O2H+IC3H7                       1.019E+001     3.580
14810.0

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

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

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

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

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

!REF:VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975
IC3H7O2+C3H8<=>IC3H7O2H+IC3H7                    2.000E+012     0.000
17000.0
C3H8+CH3CO3<=>IC3H7+CH3CO3H                      2.000E+012     0.000
17000.0

!REF:ANALOGY TO C2H6+HO2
C3H8+CH3CO3<=>NC3H7+CH3CO3H                      1.700E+013     0.000
20460.0
C3H8+O2CHO<=>NC3H7+HO2CHO                        5.520E+004     2.550
16480.0
C3H8+O2CHO<=>IC3H7+HO2CHO                        1.475E+004     2.600
13910.0

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

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

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
IC3H7+OH<=>C3H6+H2O                              2.410E+013     0.000
0.0
IC3H7+O<=>CH3COCH3+H                             4.818E+013     0.000
0.0
IC3H7+O<=>CH3CHO+CH3                             4.818E+013     0.000
0.0

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

!REF:ANALOGY WITH ACETALDEHYDE
C2H5CHO+NC3H7<=>C2H5CO+C3H8                      1.700E+012     0.000
8440.0
C2H5CHO+IC3H7<=>C2H5CO+C3H8                      1.700E+012     0.000
8440.0
C2H5CHO+C3H5-A<=>C2H5CO+C3H6                     1.700E+012     0.000
8440.0
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!REF:LASKIN ET AL. IJCK 32 589-614 2000
C2H3+CH3(+M)<=>C3H6(+M)                                 2.500E+013     0.000
0.0
LOW/                                                    4.270E+058   -11.940
9769.8/
TROE/  1.750E-001  1.341E+003  6.000E+004  1.014E+004/
C3H5-A+H(+M)<=>C3H6(+M)                                 1.000E+014     0.000
0.0
LOW/                                                    6.650E+059   -12.000
5967.8/
TROE/  2.000E-002  1.097E+003  1.097E+003  6.860E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/
C3H6<=>C3H5-S+H                                         7.710E+069   -16.090
140000.0
C3H6<=>C3H5-T+H                                         5.620E+071   -16.580
139300.0

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

!REF: ANALOGY WITH C2H4
C3H6+O<=>C2H5+HCO                                       7.450E+006     1.880
183.0
C3H6+O=>CH2CO+CH3+H                                     3.050E+006     1.880
183.0
C3H6+O=>CH3CHCO+H+H                                     3.050E+006     1.880
183.0
C3H6+O<=>C3H5-A+OH                                      5.240E+011     0.700
5884.0
C3H6+O<=>C3H5-S+OH                                      1.200E+011     0.700
8959.1
C3H6+O<=>C3H5-T+OH                                      6.030E+010     0.700
7632.0
C3H6+OH<=>C3H5-A+H2O                                    4.460E+006     2.072
1050.8
C3H6+OH<=>C3H5-S+H2O                                    1.860E+005     2.369
2502.0
C3H6+OH<=>C3H5-T+H2O                                    1.800E+006     1.979
2235.2

!REF:BILL

!REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONDARY ALKYL AND PRIMARY
ALLYLIC WITH F<=>.2: 0.2(98.4-88.2)<=>.2*10.2<=>2.0
C3H6+CH3O<=>C3H5-A+CH3OH                                8.400E+010     0.000
2600.0

!REF: C3 NUIG CALCULATION J.M
C3H6+HO2<=>C3H5-S+H2O2                                  9.570E+002     3.059
20798.6
C3H6+HO2<=>C3H5-T+H2O2                                  1.560E+004     2.820
24427.9
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C3H6+HO2<=>IC3H7O2                                  1.050E-025     3.520
5109.0
PLOG/      0.0130     8.280E+054   -14.710     21141.0/
PLOG/      0.9869     1.170E+042   -10.250     18891.0/
PLOG/      9.8700     1.170E+038    -8.770     18811.0/
PLOG/     98.6900     5.570E+022    -3.910     13896.0/
C3H6+HO2<=>C3H6OOH2-1                               4.850E-021     2.650
11201.0
PLOG/      0.0130     1.310E+013    -1.840      8561.0/
PLOG/      0.9869     5.930E+017    -2.610     11533.0/
PLOG/      9.8700     8.340E+024    -4.400     16440.0/
PLOG/     98.6900     3.750E+023    -3.680     17965.0/
C3H6+HO2<=>C3H6O1-2+OH                              1.130E+019    -1.680
23587.0
PLOG/      0.0130     3.730E+003     2.640     11173.0/
PLOG/      0.9869     1.780E+012     0.110     16137.0/
PLOG/      9.8700     3.900E+017    -1.400     20077.0/
PLOG/     98.6900     1.130E+019    -1.680     23587.0/
C3H6+HO2<=>IC3H7+O2                                 8.870E+022    -3.090
26586.0
PLOG/      0.0130     1.020E+007     1.160     10273.0/
PLOG/      0.9869     1.310E+020    -2.580     19078.0/
PLOG/      9.8700     4.140E+028    -4.920     26212.0/
PLOG/     98.6900     8.870E+022    -3.090     26586.0/
C3H6OOH2-1<=>C3H6O1-2+OH                            6.910E+007     1.370
13373.0
PLOG/      0.0130     2.660E+035    -8.360     18056.0/
PLOG/      0.9869     1.960E+035    -7.660     20595.0/
PLOG/      9.8700     2.240E+033    -6.750     21619.0/
PLOG/     98.6900     8.480E+026    -4.580     20278.0/
C3H6+HO2<=>C3H5-A+H2O2                              3.070E-002     4.403
13547.2

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

!REF: CURRAN EST
C3H6+H<=>NC3H7                                      1.000E+000     1.000
0.0
PLOG/      0.0013     7.990E+081   -23.161     22239.0/
PLOG/      0.0400     4.240E+068   -18.427     19665.0/
PLOG/      1.0000     1.040E+049   -11.500     15359.0/
PLOG/     10.0000     6.200E+041    -8.892     14637.0/
PLOG/    100.0000    -6.450E+031    -5.851      8177.8/
DUP
C3H6+H<=>NC3H7                                      1.000E+000     1.000
0.0
PLOG/      0.0013     1.850E+026    -5.830      3865.8/
PLOG/      0.0400     2.820E+030    -6.490      5470.8/
PLOG/      1.0000     3.780E+028    -5.570      5625.1/
PLOG/     10.0000     1.460E+025    -4.280      5247.8/
PLOG/    100.0000     7.240E+026    -4.210      6825.0/
DUP
C3H6+H<=>C2H4+CH3                                   1.000E+000     1.000
1.0
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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
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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/
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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/
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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/
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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/
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PLOG/      0.0130     2.870E+013     0.040     10634.0/
PLOG/      0.0250     1.590E+014    -0.160     11125.0/
PLOG/      0.1000     3.100E+014    -0.220     11407.0/
PLOG/      0.1315     3.780E+014    -0.240     11458.0/
PLOG/      1.0000     9.150E+007     1.420     10087.0/
PLOG/     10.0000     3.660E+005     2.140     10410.0/
PLOG/    100.0000     8.190E+002     2.840     10481.0/
C3H6+OH<=>C2H3OH+CH3                                 1.290E+006     1.650
1233.0
PLOG/      0.0013     1.290E+006     1.650      1233.0/
PLOG/      0.0100     1.820E+004     2.100      1162.0/
PLOG/      0.0130     2.040E+003     2.480      1128.0/
PLOG/      0.0250     2.880E+002     2.800      1152.0/
PLOG/      0.1000     1.400E+001     3.210      1208.0/
PLOG/      0.1315     7.710E+000     3.290      1216.0/
PLOG/      1.0000     1.130E+004     2.500      3238.0/
PLOG/     10.0000     2.410E+019    -1.740     13107.0/
PLOG/    100.0000     3.300E-001     3.700      3665.0/
C3H6+OH<=>IC3H5OH+H                                  2.870E+000     2.920
625.0
PLOG/      0.0013     2.870E+000     2.920       625.0/
PLOG/      0.0100     4.840E-001     2.980       704.0/
PLOG/      0.0130     3.130E-001     3.040       721.0/
PLOG/      0.0250     9.330E-003     3.620       677.0/
PLOG/      0.1000     4.640E-005     4.480       687.0/
PLOG/      0.1315     2.710E-005     4.560       707.0/
PLOG/      1.0000     7.650E-007     5.050       874.0/
PLOG/     10.0000     2.640E+015    -0.800     12728.0/
PLOG/    100.0000     4.870E-004     4.320      4020.0/
C3H6+OH<=>SC3H5OH+H                                  2.870E+000     2.920
625.0
PLOG/      0.0013     2.870E+000     2.920       625.0/
PLOG/      0.0100     4.840E-001     2.980       704.0/
PLOG/      0.0130     3.130E-001     3.040       721.0/
PLOG/      0.0250     9.330E-003     3.620       677.0/
PLOG/      0.1000     4.640E-005     4.480       687.0/
PLOG/      0.1315     2.710E-005     4.560       707.0/
PLOG/      1.0000     7.650E-007     5.050       874.0/
PLOG/     10.0000     2.640E+015    -0.800     12728.0/
PLOG/    100.0000     4.870E-004     4.320      4020.0/
C3H6+OH<=>CH3CHO+CH3                                 6.930E+005     1.490
-536.0
PLOG/      0.0013     6.930E+005     1.490      -536.0/
PLOG/      0.0100     5.940E+003     2.010      -560.0/
PLOG/      0.0130     1.100E+003     2.220      -680.0/
PLOG/      0.0250     1.070E+002     2.500      -759.0/
PLOG/      0.1000     7.830E-001     3.100      -919.0/
PLOG/      0.1315     3.070E-001     3.220      -946.0/
PLOG/      1.0000     3.160E-004     4.050     -1144.0/
PLOG/     10.0000     7.590E-006     4.490      -680.0/
PLOG/    100.0000     5.450E-005     4.220      1141.0/
C3H6+OH<=>C3H6OH1-2                                  5.100E+054   -20.700
32402.0
PLOG/      0.0013     2.300E+078   -20.700     32402.0/
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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)
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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 SECONARY ALKYL AND PRIMARY
ALLYLIC WITH F<=>.2: 0.2(98.4-88.2)<=>.2*10.2<=>2.0

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

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

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

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

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

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

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

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589
C2H2+CH3<=>C3H5-A                                  8.200E+053   -13.320
33200.0
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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
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!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
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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
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!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/
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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                                7.300E+012     0.000
2250.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H4-P+O<=>C2H4+CO                                 1.000E+013     0.000
2250.0


!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H4-P+C2H<=>C2H2+C3H3                             1.000E+013     0.000
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H4-P+CH3<=>C3H3+CH4                              1.800E+012     0.000
7700.0



!REF:PITZ ESTIMATE
C2H+CH3<=>C3H4-P                                   8.000E+013     0.000
0.0

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

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H4-P+HO2=>C2H4+CO+OH                             3.000E+012     0.000
19000.0

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H4-P+O<=>C2H3+HCO                                3.200E+012     0.000
2010.0

!REF:GLAUDE,P.A. ET AL,PROC. COMBUST. INST
C3H4-P+O<=>C3H3+OH                                 7.650E+008     1.500
8600.0

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H4-P+C2H3<=>C3H3+C2H4                            1.000E+012     0.000
7700.0
C3H4-P+C3H5-A<=>C3H3+C3H6                          3.000E+012     0.000
7700.0
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!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H3+O<=>CH2O+C2H                                 2.000E+013     0.000
0.0

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

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H3+HO2=>OH+CO+C2H3                              8.000E+011     0.000
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H3+HCO<=>C3H4-A+CO                              2.500E+013     0.000
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H3+HCO<=>C3H4-P+CO                              2.500E+013     0.000
0.0

!REF:
C2H5+C2H<=>C3H3+CH3                               1.810E+013     0.000
0.0

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H4-A+HO2=>C2H4+CO+OH                            1.000E+011     0.000
14000.0
C3H4-A+HO2<=>C3H3+H2O2                            3.580E-002     4.170
9632.8
C3H4-A+CH3O2<=>C3H3+CH3O2H                        7.161E-002     4.170
9632.8
C3H4-P+HO2<=>C3H3+H2O2                            9.550E-002     4.170
9632.8
C3H4-P+CH3O2<=>C3H3+CH3O2H                        9.550E-002     4.170
9632.8

!REF: ESTIMATE ATKINSON 1984 C3 NUIG S.M.B
C3H4-A+OH<=>CH2CCH2OH                             1.110E+012     0.000
-304.0
C3H4-A+OH<=>SC3H4OH                               2.220E+012     0.000
-304.0

!REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP
CH2CCH2OH<=>CH2O+C2H3                             9.240E+010     0.870
30460.0
CH2CCH2OH<=>C2H3CHO+H                             1.110E+011     0.480
36770.0
CH2CCH2OH<=>HCO+C2H4                              9.240E+010     0.870
30460.0
SC3H4OH<=>CH2CO+CH3                               9.240E+010     0.870
30460.0
C3H4-A+H<=>C3H3+H2                                6.625E+003     3.095
5522.0

!REF: ANALOGIES WITH C3H6 A AND S
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C3H4-P+OH<=>C3H3+H2O                                4.940E+006     2.027
1059.6
C3H4-A+OH<=>C3H3+H2O                                1.482E+005     2.492
1807.2
C3H4-P+H<=>C3H3+H2                                  3.572E+004     2.825
4821.0

!REF: ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984
C3H4-P+OH<=>PC3H4OH-2                               3.930E+011     0.000
0.0
C3H4-P+OH<=>SC3H4OH                                 2.360E+012     0.000
0.0

!REF: MATHEU ET AL. IJCK, 2003, 35, 95--119
PC3H4OH-2<=>CH3CHCHO                                3.560E+010     0.880
23238.0

!REF: PELUCCHI ECM 2013
CH3CHCHO<=>C2H3CHO+H                                4.164E+012    -0.020
32410.0
CH3CHCHO<=>CH3CHCO+H                                8.328E+012    -0.020
32410.0
C3H3+H<=>C3H2+H2                                    2.140E+005     2.520
7453.0
C3H3+H<=>C3H2(S)+H2                                 3.311E+013     0.195
17579.0
PLOG/      0.0395     2.951E+009     1.280     13474.0/
PLOG/      1.0000     1.097E+010     1.130     13929.0/
PLOG/     10.0000     3.311E+013     0.195     17579.0/
C3H3+H<=>H2CCC(S)+H2                                1.000E+018    -1.230
15111.0
PLOG/      0.0395     2.692E+009     1.050      5371.0/
PLOG/      1.0000     2.884E+013    -0.030      9448.0/
PLOG/     10.0000     1.000E+018    -1.230     15111.0/
C3H3+H<=>C3H2C+H2                                   7.244E+009     0.606
18356.0
PLOG/      0.0395     1.072E+007     1.370     15557.0/
PLOG/      1.0000     1.349E+007     1.340     15560.0/
PLOG/     10.0000     7.244E+009     0.606     18356.0/
C3H4-A<=>C3H4-P                                     4.786E+048   -10.000
88685.0
PLOG/      1.0000     7.762E+039    -7.800     78446.0/
PLOG/     10.0000     4.786E+048   -10.000     88685.0/
CC3H4<=>C3H4-P                                      1.660E+037    -7.240
48013.0
PLOG/      0.0395     2.512E+050   -11.820     50914.0/
PLOG/      1.0000     1.230E+037    -7.510     45551.0/
PLOG/     10.0000     1.660E+037    -7.240     48013.0/
CC3H4<=>C3H4-A                                      5.012E+035    -6.870
51298.0
PLOG/      0.0395     9.772E+043    -9.970     56007.0/
PLOG/      1.0000     2.512E+026    -4.560     43922.0/
PLOG/     10.0000     5.012E+035    -6.870     51298.0/
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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
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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/
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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
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!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:
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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                       1.130E+013     0.000
30430.0

!REF:ANALOGY TO CH3OH+HO2
CH3OH+NC3H7O2<=>CH2OH+NC3H7O2H                     6.300E+012     0.000
19360.0
CH3OH+IC3H7O2<=>CH2OH+IC3H7O2H                     6.300E+012     0.000
19360.0

!REF:HALF OF CH2O+HO2
C2H3CHO+NC3H7O2<=>C2H3CO+NC3H7O2H                  2.800E+012     0.000
13600.0
C2H3CHO+IC3H7O2<=>C2H3CO+IC3H7O2H                  2.800E+012     0.000
13600.0
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!REF:ANALOGY TO CH4+HO2
CH4+NC3H7O2<=>CH3+NC3H7O2H                          1.120E+013     0.000
24640.0
CH4+IC3H7O2<=>CH3+IC3H7O2H                          1.120E+013     0.000
24640.0

!REF:
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2                       1.400E+016    -1.610
1860.0
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2                       1.400E+016    -1.610
1860.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)
H2+NC3H7O2<=>H+NC3H7O2H                             3.010E+013     0.000
26030.0
H2+IC3H7O2<=>H+IC3H7O2H                             3.010E+013     0.000
26030.0

!REF:WESTBROOK ESTIMATE
IC3H7O2+C2H6<=>IC3H7O2H+C2H5                        1.700E+013     0.000
20460.0
NC3H7O2+C2H6<=>NC3H7O2H+C2H5                        1.700E+013     0.000
20460.0
IC3H7O2+C2H5CHO<=>IC3H7O2H+C2H5CO                   2.000E+011     0.000
9500.0
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO                   2.000E+011     0.000
9500.0

!REF:
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2                    1.400E+016    -1.610
1860.0
NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2                    1.400E+016    -1.610
1860.0
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2                     1.400E+016    -1.610
1860.0
NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2                     1.400E+016    -1.610
1860.0
IC3H7O2+IC3H7O2=>O2+IC3H7O+IC3H7O                   1.400E+016    -1.610
1860.0
NC3H7O2+NC3H7O2=>O2+NC3H7O+NC3H7O                   1.400E+016    -1.610
1860.0
IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2                   1.400E+016    -1.610
1860.0
IC3H7O2+CH3<=>IC3H7O+CH3O                           7.000E+012     0.000
-1000.0
IC3H7O2+C2H5<=>IC3H7O+C2H5O                         7.000E+012     0.000
-1000.0
IC3H7O2+IC3H7<=>IC3H7O+IC3H7O                       7.000E+012     0.000
-1000.0
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O                       7.000E+012     0.000
-1000.0
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O                       7.000E+012     0.000
-1000.0
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NC3H7O2+CH3<=>NC3H7O+CH3O                          7.000E+012     0.000
-1000.0
NC3H7O2+C2H5<=>NC3H7O+C2H5O                        7.000E+012     0.000
-1000.0
NC3H7O2+IC3H7<=>NC3H7O+IC3H7O                      7.000E+012     0.000
-1000.0
NC3H7O2+NC3H7<=>NC3H7O+NC3H7O                      7.000E+012     0.000
-1000.0
NC3H7O2+C3H5-A<=>NC3H7O+C3H5O                      7.000E+012     0.000
-1000.0
NC3H7O2H<=>NC3H7O+OH                               1.500E+016     0.000
42500.0

!REF:PITZ ESTIMATE
IC3H7O+OH<=>IC3H7O2H                               1.000E+015    -0.800
0.0

!REF:
C2H5+CH2O<=>NC3H7O                                 1.000E+011     0.000
3496.0
C2H5CHO+H<=>NC3H7O                                 4.000E+012     0.000
6260.0
CH3+CH3CHO<=>IC3H7O                                1.000E+011     0.000
9256.0
CH3COCH3+H<=>IC3H7O                                2.000E+012     0.000
7270.0

!REF:BALLA ET AL., CHEM. PHYSICS, 99, 323 (1985)
IC3H7O+O2<=>CH3COCH3+HO2                           9.090E+009     0.000
390.0

!REF:
NC3H7O2<=>C3H6OOH1-2                              6.000E+011     0.000
26850.0
NC3H7O2<=>C3H6OOH1-3                              1.125E+011     0.000
24400.0
IC3H7O2<=>C3H6OOH2-1                              1.800E+012     0.000
29400.0

!REF:BOZZELLI, J. AND DEAN, A, 1992
IC3H7O2<=>C3H6OOH2-2                              1.230E+035    -6.960
48880.0

!REF:
C3H6OOH1-2<=>C3H6O1-2+OH                          6.000E+011     0.000
22000.0
C3H6OOH1-3<=>C3H6O1-3+OH                          7.500E+010     0.000
15250.0

!REF:
C3H6+HO2<=>C3H6OOH1-2                             1.000E+011     0.000
11000.0
C3H6OOH1-3=>OH+CH2O+C2H4                          3.035E+015    -0.790
27400.0
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!REF:BOZZELLI AND PITZ, 1995
C3H6OOH2-1<=>C2H3OOH+CH3                          6.540E+027    -5.140
38320.0
C3H6OOH1-2=>C2H4+CH2O+OH                          1.310E+033    -7.010
48120.0

!REF:ESTIMATE
C3H6OOH2-2<=>CH3COCH3+OH                          9.000E+014     0.000
1500.0
C3H6OOH1-2+O2<=>C3H6OOH1-2O2                      5.000E+012     0.000
0.0
C3H6OOH1-3+O2<=>C3H6OOH1-3O2                      4.520E+012     0.000
0.0
C3H6OOH2-1+O2<=>C3H6OOH2-1O2                      4.520E+012     0.000
0.0

!REF:
C3H6OOH1-2O2<=>C3KET12+OH                         6.000E+011     0.000
26400.0
C3H6OOH1-3O2<=>C3KET13+OH                         7.500E+010     0.000
21400.0
C3H6OOH2-1O2<=>C3KET21+OH                         3.000E+011     0.000
23850.0
C3H6OOH2-1O2<=>C3H51-2,3OOH                       1.125E+011     0.000
24400.0
C3H6OOH1-2O2<=>C3H51-2,3OOH                       9.000E+011     0.000
29400.0

!REF: BOZZELLI AND PITZ, 1993.
C3H51-2,3OOH<=>AC3H5OOH+HO2                       2.560E+013    -0.490
17770.0

!REF:
C3H6OOH1-3O2<=>C3H52-1,3OOH                       6.000E+011     0.000
26850.0

!REF:BOZZELLI AND PITZ, 1993.
C3H52-1,3OOH<=>AC3H5OOH+HO2                       1.150E+014    -0.630
17250.0

!REF:
C3KET12=>CH3CHO+HCO+OH                            9.450E+015     0.000
43000.0
C3KET13=>CH2O+CH2CHO+OH                           1.000E+016     0.000
43000.0
C3KET21=>CH2O+CH3CO+OH                            1.000E+016     0.000
43000.0

!REF:ESTIMATE

!REF:

!REF:ACETALDEHYDE ANALOG
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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/
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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)
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C4H10+O<=>PC4H9+OH                                1.130E+014     0.000
7850.0
C4H10+O<=>SC4H9+OH                                5.620E+013     0.000
5200.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-
7054.
C4H10+HO2<=>PC4H9+H2O2                            4.080E+001     3.590
17160.0
C4H10+HO2<=>SC4H9+H2O2                            1.264E+002     3.370
13720.0

!REF:DRYER ESTIMATE
C4H10+CH3O<=>PC4H9+CH3OH                          3.000E+011     0.000
7000.0
C4H10+CH3O<=>SC4H9+CH3OH                          6.000E+011     0.000
7000.0

!REF:ANOLOGY TO CH3O
C4H10+C2H5O<=>PC4H9+C2H5OH                        3.000E+011     0.000
7000.0
C4H10+C2H5O<=>SC4H9+C2H5OH                        6.000E+011     0.000
7000.0

!REF:!WESTBROOK AND PITZ ESTIMATE (1983)
C4H10+PC4H9<=>SC4H9+C4H10                         1.000E+011     0.000
10400.0

!REF:ANALOGY TO C2H6+HO2
C4H10+CH3CO3<=>PC4H9+CH3CO3H                      1.700E+013     0.000
20460.0

!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
!REF:SEATTLE, AUGUST, 1988
C4H10+CH3CO3<=>SC4H9+CH3CO3H                      1.120E+013     0.000
17700.0

!REF:ANALOGY WITH RH+RO2 --> R+RO2H
C4H10+O2CHO<=>PC4H9+HO2CHO                        1.680E+013     0.000
20440.0
C4H10+O2CHO<=>SC4H9+HO2CHO                        1.120E+013     0.000
17690.0

!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                        1.386E+000     3.970
18280.0
CH3O2+C4H10<=>CH3O2H+SC4H9                        2.037E+001     3.580
14810.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-
7054.
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C2H5O2+C4H10<=>C2H5O2H+PC4H9                      4.080E+001     3.590
17160.0
C2H5O2+C4H10<=>C2H5O2H+SC4H9                      1.264E+002     3.370
13720.0

!REF:ANALOGY TO C2H6+HO2
NC3H7O2+C4H10<=>NC3H7O2H+PC4H9                    1.700E+013     0.000
20460.0

!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
!REF:SEATTLE, AUGUST, 1988
NC3H7O2+C4H10<=>NC3H7O2H+SC4H9                    1.120E+013     0.000
17700.0

!REF:ANALOGY TO C2H6+HO2
IC3H7O2+C4H10<=>IC3H7O2H+PC4H9                    1.700E+013     0.000
20460.0

!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
!REF:SEATTLE, AUGUST, 1988
IC3H7O2+C4H10<=>IC3H7O2H+SC4H9                    1.120E+013     0.000
17700.0

!REF:ANALOGY TO C2H6+HO2
PC4H9O2+C3H8<=>PC4H9O2H+NC3H7                     1.700E+013     0.000
20460.0

!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY,
1975
PC4H9O2+C3H8<=>PC4H9O2H+IC3H7                     2.000E+012     0.000
17000.0

!REF:ANALOGY TO C2H6+HO2
PC4H9O2+C4H10<=>PC4H9O2H+PC4H9                    1.700E+013     0.000
20460.0

!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
!REF:SEATTLE, AUGUST, 1988
PC4H9O2+C4H10<=>PC4H9O2H+SC4H9                    1.120E+013     0.000
17700.0

!REF:ANALOGY TO C2H6+HO2
SC4H9O2+C3H8<=>SC4H9O2H+NC3H7                     1.700E+013     0.000
20460.0

!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY,
1975
SC4H9O2+C3H8<=>SC4H9O2H+IC3H7                     2.000E+012     0.000
17000.0
SC4H9O2+C4H10<=>SC4H9O2H+PC4H9                    1.700E+013     0.000
20460.0

!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION
 !REF:SEATTLE, AUGUST, 1988
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SC4H9O2+C4H10<=>SC4H9O2H+SC4H9                    1.120E+013     0.000
17700.0

!REF:D.M. MATHEU, W.H. GREEN JR., J.M. GRENDA, INT. J. CHEM. KINET. 35
(2003) 95-119.
PC4H9<=>SC4H9                                     3.560E+010     0.880
37300.0
DUP
PC4H9<=>SC4H9                                     3.800E+010     0.670
36600.0
DUP

!REF:
C2H5+C2H4<=>PC4H9                                 1.320E+004     2.480
6130.0
C3H6+CH3<=>SC4H9                                  1.760E+004     2.480
6130.0
C4H8-1+H<=>PC4H9                                  2.500E+011     0.510
2620.0
C4H8-2+H<=>SC4H9                                  2.500E+011     0.510
2620.0
C4H8-1+H<=>SC4H9                                  4.240E+011     0.510
1230.0

!REF:BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2
PC4H9+O2<=>C4H8-1+HO2                             8.370E-001     3.590
11960.0
SC4H9+O2<=>C4H8-1+HO2                             5.350E-001     3.710
9322.0
SC4H9+O2<=>C4H8-2+HO2                             1.070E+000     3.710
9322.0

!REF:WESTBROOK AND PITZ ESTIMATE (1983).
C2H3+C2H5<=>C4H8-1                                9.000E+012     0.000
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-A+CH3(+M)<=>C4H8-1(+M)                       1.000E+014    -0.320
-262.3
LOW/                                              3.910E+060   -12.810
6250.0/
TROE/  1.040E-001  1.606E+003  6.000E+004  6.118E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/

!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
H+C4H71-3<=>C4H8-1                                5.000E+013     0.000
0.0

!REF:ESTIMATE
C4H8-1+O2<=>C4H71-3+HO2                           2.000E+013     0.000
37190.0

!REF:
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C4H8-1+O<=>C4H71-3+OH                                1.750E+011     0.700
5884.0
C4H8-2+O<=>C4H71-3+OH                                2.190E+011     0.810
7550.0

!REF:TSANG '91
C4H8-1+H<=>C4H71-3+H2                                1.730E+005     2.500
2492.0

!REF:ESTIMATE
C4H8-1+H<=>C4H71-4+H2                                6.651E+005     2.540
6756.0
C4H8-1+OH<=>C4H71-1+H2O                              9.010E-001     3.941
1637.9
C4H8-1+OH<=>C4H71-2+H2O                              1.430E+001     3.534
478.1
C4H8-1+OH<=>C4H71-3+H2O                              6.690E+001     3.475
-2802.5
C4H8-1+OH<=>C4H71-4+H2O                              4.280E+001     3.374
-767.0

!REF:BASED ON 0.5 * C2H4+OH<=>C2H3+H2O
!REF:ESTIMATE
!REF:TSANG '91
!REF:TSANG '91
C4H8-1+CH3<=>C4H71-3+CH4                             2.210E+000     3.500
5675.0
C4H8-1+CH3<=>C4H71-4+CH4                             4.520E-001     3.650
7154.0

!REF:TSANG '91
C4H8-1+HO2<=>C4H71-3+H2O2                            2.700E+004     0.700
5884.0
C4H8-1+HO2<=>C4H71-4+H2O2                            2.380E+003     2.550
16490.0

!REF:TSANG '91
C4H8-1+CH3O2<=>C4H71-3+CH3O2H                        2.700E+004     0.700
5884.0
C4H8-1+CH3O2<=>C4H71-4+CH3O2H                        2.380E+003     2.550
16490.0
C4H8-1+CH3O<=>C4H71-3+CH3OH                          4.000E+001     2.900
8609.0
C4H8-1+CH3O<=>C4H71-4+CH3OH                          2.170E+011     0.000
6458.0

!REF:DECHAUX, J.C., OXID. COMM. 2, 95 (1981)
C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H                      1.000E+011     0.000
8000.0
C4H8-1+C3H5-A<=>C4H71-3+C3H6                         7.900E+010     0.000
12400.0

!REF:ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).
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C4H71-3+C4H71-3<=>C4H8-1+C4H6                      1.600E+012     0.000
0.0
C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H                    1.400E+012     0.000
14900.0
C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H                  1.400E+012     0.000
14900.0
C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H                  1.400E+012     0.000
14900.0
C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H                  1.400E+012     0.000
14900.0
C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H                  1.400E+012     0.000
14900.0
C4H8-1+CH3O2<=>C4H8O1-2+CH3O                       1.000E+012     0.000
14340.0

!REF:ALLARA AND SHAW, 1980, PARALLEL
H+C4H71-3<=>C4H8-2                                 5.000E+013     0.000
0.0
C4H8-2+O2<=>C4H71-3+HO2                            4.000E+013     0.000
39390.0

!REF:TSANG '91

!REF:PLUS DIFFERENCE BETWEEN 1O AND 2O 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
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!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                      1.000E+016     0.000
25000.0
C2H2+C2H5<=>C4H71-1                               2.000E+011     0.000
7800.0
C3H4-A+CH3<=>C4H71-2                              2.000E+011     0.000
7800.0
C2H4+C2H3<=>C4H71-4                               2.000E+011     0.000
7800.0
C3H4-P+CH3<=>C4H72-2                              1.000E+011     0.000
7800.0

!REF:!ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
C4H6+H<=>C4H71-3                                  4.000E+013     0.000
1300.0

!REF:ESTIMATE
C4H71-3+C2H5<=>C4H8-1+C2H4                        2.590E+012     0.000
-131.0
C4H71-3+CH3O<=>C4H8-1+CH2O                        2.410E+013     0.000
0.0
C4H71-3+O<=>C2H3CHO+CH3                           6.030E+013     0.000
0.0
C4H71-3+HO2<=>C4H7O+OH                            9.640E+012     0.000
0.0
C4H71-3+CH3O2<=>C4H7O+CH3O                        9.640E+012     0.000
0.0

!REF:EDELSON AND ALLARA, 1980
C3H5-A+C4H71-3<=>C3H6+C4H6                        6.310E+012     0.000
0.0

!REF:BALDWIN, BENNETT, AND WALKER, JCS FARADAY I, 76, 2396 (1980)
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C4H71-3+O2<=>C4H6+HO2                                1.000E+009     0.000
0.0

!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
H+C4H71-3<=>C4H6+H2                                  3.160E+013     0.000
0.0

!REF:EDELSON AND ALLARA, 1980
C2H5+C4H71-3<=>C4H6+C2H6                             3.980E+012     0.000
0.0
C2H3+C4H71-3<=>C2H4+C4H6                             3.980E+012     0.000
0.0

!REF:ANALOGY TO CH3O2+CH3
C4H71-3+C2H5O2<=>C4H7O+C2H5O                         3.800E+012     0.000
-1200.0
IC3H7O2+C4H71-3<=>IC3H7O+C4H7O                       3.800E+012     0.000
-1200.0
NC3H7O2+C4H71-3<=>NC3H7O+C4H7O                       3.800E+012     0.000
-1200.0

!REF:ANALOGY TO BATT'S RATE FOR S-BUTOXY DECOMPOSITION
C4H7O<=>CH3CHO+C2H3                                  7.940E+014     0.000
19000.0
C4H7O<=>C2H3CHO+CH3                                  7.940E+014     0.000
19000.0

!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
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!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/
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C2H3+C2H2<=>C4H5-I                                  5.000E+034    -8.420
7900.0
PLOG/      0.0132     5.000E+034    -8.420      7900.0/
PLOG/      0.0263     2.100E+036    -8.780      9100.0/
PLOG/      0.1200     1.000E+037    -8.770      9800.0/
PLOG/      1.0000     1.600E+046   -10.980     18600.0/
PLOG/     10.0000     5.100E+053   -12.640     28800.0/
C2H3+C2H3<=>C4H6                                    7.000E+057   -13.820
17629.0
PLOG/      0.0263     7.000E+057   -13.820     17629.0/
PLOG/      0.1200     1.500E+052   -11.970     16056.0/
PLOG/      1.0000     1.500E+042    -8.840     12483.0/
C2H3+C2H3<=>C4H5-I+H                                1.500E+030    -4.950
12958.0
PLOG/      0.0263     1.500E+030    -4.950     12958.0/
PLOG/      0.1200     7.200E+028    -4.490     14273.0/
PLOG/      1.0000     1.200E+022    -2.440     13654.0/
C2H3+C2H3<=>C4H5-N+H                                1.100E+024    -3.280
12395.0
PLOG/      0.0263     1.100E+024    -3.280     12395.0/
PLOG/      0.1200     4.600E+024    -3.380     14650.0/
PLOG/      1.0000     2.400E+020    -2.040     15361.0/
C4H5-N<=>C4H5-I                                     2.400E+060   -16.080
47500.0
PLOG/      0.0132     2.400E+060   -16.080     47500.0/
PLOG/      0.0263     1.300E+062   -16.380     49600.0/
PLOG/      0.1200     4.900E+066   -17.260     55400.0/
PLOG/      1.0000     1.500E+067   -16.890     59100.0/
PLOG/     10.0000     2.000E+060   -14.460     58600.0/
C4H5-N+H<=>C4H5-I+H                                 3.100E+026    -3.350
17423.0
C4H5-N+H<=>C4H4+H2                                  1.500E+013     0.000
0.0
C4H5-N+OH<=>C4H4+H2O                                2.000E+012     0.000
0.0
C4H5-N+HCO<=>C4H6+CO                                5.000E+012     0.000
0.0
C4H5-N+HO2=>C2H3+CH2CO+OH                           6.600E+012     0.000
0.0
C4H5-N+H2O2<=>C4H6+HO2                              1.210E+010     0.000
-596.0
C4H5-N+HO2<=>C4H6+O2                                6.000E+011     0.000
0.0
C4H5-N+O2<=>CH2CHCHCHO+O                            3.000E+011     0.290
11.0
C4H5-N+O2<=>HCO+C2H3CHO                             9.200E+016    -1.390
1010.0
C4H5-I+H<=>C4H4+H2                                  3.000E+013     0.000
0.0
C4H5-I+H<=>C3H3+CH3                                 2.000E+013     0.000
2000.0
C4H5-I+OH<=>C4H4+H2O                                4.000E+012     0.000
0.0
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C4H5-I+HCO<=>C4H6+CO                              5.000E+012     0.000
0.0
C4H5-I+HO2<=>C4H6+O2                              6.000E+011     0.000
0.0
C4H5-I+HO2=>C2H3+CH2CO+OH                         6.600E+012     0.000
0.0
C4H5-I+H2O2<=>C4H6+HO2                            1.210E+010     0.000
-596.0
C4H5-I+O2<=>CH2CO+CH2CHO                          2.160E+010     0.000
2500.0
C4H5-2<=>C4H5-I                                   1.500E+067   -16.890
59100.0
C4H5-2+H<=>C4H5-I+H                               3.100E+026    -3.350
17423.0
C4H5-2+HO2=>OH+C2H2+CH3CO                         8.000E+011     0.000
0.0
C4H5-2+O2<=>CH3CO+CH2CO                           2.160E+010     0.000
2500.0
C4H612<=>C4H5-I+H                                 4.200E+015     0.000
92600.0
C4H612+H<=>C4H6+H                                 2.000E+013     0.000
4000.0
C4H612+H<=>C4H5-I+H2                              1.700E+005     2.500
2490.0
C4H612+H<=>C3H4-A+CH3                             2.000E+013     0.000
2000.0
C4H612+H<=>C3H4-P+CH3                             2.000E+013     0.000
2000.0
C4H612+CH3<=>C4H5-I+CH4                           7.000E+013     0.000
18500.0
C4H612+O<=>CH2CO+C2H4                             1.200E+008     1.650
327.0
C4H612+O<=>C4H5-I+OH                              1.800E+011     0.700
5880.0
C4H612+OH<=>C4H5-I+H2O                            3.100E+006     2.000
-298.0
C4H612<=>C4H6                                     3.000E+013     0.000
65000.0
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
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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
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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
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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                          5.000E+012     0.000
0.0
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2                      1.000E+013     0.000
15000.0
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C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H                1.000E+013     0.000
19000.0
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4                     2.000E+011     0.000
10000.0
C4H8O1-4+OH=>CH2O+C3H5-A+H2O                      5.000E+012     0.000
0.0
C4H8O1-4+H=>CH2O+C3H5-A+H2                        5.000E+012     0.000
0.0
C4H8O1-4+O=>CH2O+C3H5-A+OH                        5.000E+012     0.000
0.0
C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2                    1.000E+013     0.000
15000.0
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H                1.000E+013     0.000
19000.0
C4H8O1-4+CH3=>CH2O+C3H5-A+CH4                     2.000E+011     0.000
10000.0
C4H8O2-3+OH=>CH2O+C3H5-A+H2O                      5.000E+012     0.000
0.0
C4H8O2-3+H=>CH2O+C3H5-A+H2                        5.000E+012     0.000
0.0
C4H8O2-3+O=>CH2O+C3H5-A+OH                        5.000E+012     0.000
0.0
C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2                    1.000E+013     0.000
15000.0
C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H                1.000E+013     0.000
19000.0
C4H8O2-3+CH3=>CH2O+C3H5-A+CH4                     2.000E+011     0.000
10000.0

!REF:ESTIMATE
PC4H9+O2<=>PC4H9O2                                4.520E+012     0.000
0.0
SC4H9+O2<=>SC4H9O2                                7.540E+012     0.000
0.0

!REF:ANALOGY TO CH2O+HO2
SC4H9O2+CH2O<=>SC4H9O2H+HCO                       5.600E+012     0.000
13600.0
SC4H9O2+CH3CHO<=>SC4H9O2H+CH3CO                   2.800E+012     0.000
13600.0

!REF:ESTIMATE
SC4H9O2+HO2<=>SC4H9O2H+O2                         1.750E+010     0.000
-3275.0
IC3H7O2+PC4H9<=>IC3H7O+PC4H9O                     7.000E+012     0.000
-1000.0
IC3H7O2+SC4H9<=>IC3H7O+SC4H9O                     7.000E+012     0.000
-1000.0
NC3H7O2+PC4H9<=>NC3H7O+PC4H9O                     7.000E+012     0.000
-1000.0
NC3H7O2+SC4H9<=>NC3H7O+SC4H9O                     7.000E+012     0.000
-1000.0
SC4H9O2+SC4H9O2=>O2+SC4H9O+SC4H9O                 1.400E+016    -1.610
1860.0
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SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2                 1.400E+016    -1.610
1860.0
SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2                 1.400E+016    -1.610
1860.0
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2                   1.400E+016    -1.610
1860.0
SC4H9O2+CH3O2=>SC4H9O+CH3O+O2                     1.400E+016    -1.610
1860.0
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2                  1.400E+016    -1.610
1860.0

!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986
H2+PC4H9O2<=>H+PC4H9O2H                           3.010E+013     0.000
26030.0
H2+SC4H9O2<=>H+SC4H9O2H                           3.010E+013     0.000
26030.0

!REF:WESTBROOK ESTIMATE
C2H6+PC4H9O2<=>C2H5+PC4H9O2H                      1.700E+013     0.000
20460.0
C2H6+SC4H9O2<=>C2H5+SC4H9O2H                      1.700E+013     0.000
20460.0
PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO                 2.000E+011     0.000
9500.0
SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO                 2.000E+011     0.000
9500.0

!REF:ESTIMATE
SC4H9O2+CH3<=>SC4H9O+CH3O                         7.000E+012     0.000
-1000.0
SC4H9O2+C2H5<=>SC4H9O+C2H5O                       7.000E+012     0.000
-1000.0
SC4H9O2+IC3H7<=>SC4H9O+IC3H7O                     7.000E+012     0.000
-1000.0
SC4H9O2+NC3H7<=>SC4H9O+NC3H7O                     7.000E+012     0.000
-1000.0
SC4H9O2+PC4H9<=>SC4H9O+PC4H9O                     7.000E+012     0.000
-1000.0
SC4H9O2+SC4H9<=>SC4H9O+SC4H9O                     7.000E+012     0.000
-1000.0
SC4H9O2+C3H5-A<=>SC4H9O+C3H5O                     7.000E+012     0.000
-1000.0

!REF:ANALOGY TO CH2O+HO2
PC4H9O2+CH2O<=>PC4H9O2H+HCO                       5.600E+012     0.000
13600.0

!REF:HALF OF CH2O+HO2
PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO                   2.800E+012     0.000
13600.0

!REF:TSANG, JPC REF. DATA, 16:471 (1987)
PC4H9O2+HO2<=>PC4H9O2H+O2                         1.750E+010     0.000
-3275.0
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!REF:ANALOGY TO C3H6+HO2
C3H6+PC4H9O2<=>C3H5-A+PC4H9O2H                    5.350E-002     4.207
13288.1
C3H6+SC4H9O2<=>C3H5-A+SC4H9O2H                    5.350E-002     4.207
13288.1

!REF:ANALOGY TO C2H4+HO2
C2H4+PC4H9O2<=>C2H3+PC4H9O2H                      1.130E+013     0.000
30430.0
C2H4+SC4H9O2<=>C2H3+SC4H9O2H                      1.130E+013     0.000
30430.0

!REF:ANALOGY TO CH3OH+HO2
CH3OH+PC4H9O2<=>CH2OH+PC4H9O2H                    6.300E+012     0.000
19360.0
CH3OH+SC4H9O2<=>CH2OH+SC4H9O2H                    6.300E+012     0.000
19360.0

!REF:HALF OF CH2O+HO2
C2H3CHO+PC4H9O2<=>C2H3CO+PC4H9O2H                 2.800E+012     0.000
13600.0
C2H3CHO+SC4H9O2<=>C2H3CO+SC4H9O2H                 2.800E+012     0.000
13600.0

!REF:ANALOGY TO CH4+HO2
CH4+PC4H9O2<=>CH3+PC4H9O2H                        1.120E+013     0.000
24640.0
CH4+SC4H9O2<=>CH3+SC4H9O2H                        1.120E+013     0.000
24640.0

!REF:ESTIMATE
C4H71-3+PC4H9O2<=>C4H7O+PC4H9O                    7.000E+012     0.000
-1000.0
C4H71-3+SC4H9O2<=>C4H7O+SC4H9O                    7.000E+012     0.000
-1000.0

!REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H
H2O2+PC4H9O2<=>HO2+PC4H9O2H                       2.400E+012     0.000
10000.0
H2O2+SC4H9O2<=>HO2+SC4H9O2H                       2.400E+012     0.000
10000.0

!REF:
PC4H9O2+PC4H9O2=>O2+PC4H9O+PC4H9O                 1.400E+016    -1.610
1860.0
PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2                 1.400E+016    -1.610
1860.0
PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2                 1.400E+016    -1.610
1860.0
PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2                 1.400E+016    -1.610
1860.0
PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2                   1.400E+016    -1.610
1860.0
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PC4H9O2+CH3O2=>PC4H9O+CH3O+O2                    1.400E+016    -1.610
1860.0
PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2                 1.400E+016    -1.610
1860.0

!REF:ESTIMATE
PC4H9O2+CH3<=>PC4H9O+CH3O                        7.000E+012     0.000
-1000.0
PC4H9O2+C2H5<=>PC4H9O+C2H5O                      7.000E+012     0.000
-1000.0
PC4H9O2+IC3H7<=>PC4H9O+IC3H7O                    7.000E+012     0.000
-1000.0
PC4H9O2+NC3H7<=>PC4H9O+NC3H7O                    7.000E+012     0.000
-1000.0
PC4H9O2+PC4H9<=>PC4H9O+PC4H9O                    7.000E+012     0.000
-1000.0
PC4H9O2+SC4H9<=>PC4H9O+SC4H9O                    7.000E+012     0.000
-1000.0
PC4H9O2+C3H5-A<=>PC4H9O+C3H5O                    7.000E+012     0.000
-1000.0
PC4H9+HO2<=>PC4H9O+OH                            7.000E+012     0.000
-1000.0
SC4H9+HO2<=>SC4H9O+OH                            7.000E+012     0.000
-1000.0
CH3O2+PC4H9<=>CH3O+PC4H9O                        7.000E+012     0.000
-1000.0
CH3O2+SC4H9<=>CH3O+SC4H9O                        7.000E+012     0.000
-1000.0

!REF:
PC4H9O2H<=>PC4H9O+OH                             1.500E+016     0.000
42500.0

!REF:PITZ ESTIMATE
SC4H9O+OH<=>SC4H9O2H                             1.000E+015    -0.800
0.0

!REF:
NC3H7+CH2O<=>PC4H9O                              5.000E+010     0.000
3457.0
CH3+C2H5CHO<=>SC4H9O                             5.000E+010     0.000
9043.0
C2H5+CH3CHO<=>SC4H9O                             3.330E+010     0.000
6397.0

!REF:
PC4H9O2<=>C4H8OOH1-2                             2.000E+011     0.000
31850.0
PC4H9O2<=>C4H8OOH1-3                             2.500E+010     0.000
20850.0
PC4H9O2<=>C4H8OOH1-4                             4.688E+009     0.000
22350.0
SC4H9O2<=>C4H8OOH2-1                             3.000E+011     0.000
34500.0
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SC4H9O2<=>C4H8OOH2-3                              2.000E+011     0.000
31850.0
SC4H9O2<=>C4H8OOH2-4                              3.750E+010     0.000
24400.0
PC4H9O2<=>C4H8-1+HO2                              4.308E+036    -7.500
39510.0
SC4H9O2<=>C4H8-1+HO2                              5.980E+042    -9.430
41530.0
SC4H9O2<=>C4H8-2+HO2                              4.308E+036    -7.500
39510.0

!REF:
C4H8-1+HO2<=>C4H8OOH1-2                           1.000E+011     0.000
11000.0
C4H8-1+HO2<=>C4H8OOH2-1                           1.000E+011     0.000
11750.0
C4H8-2+HO2<=>C4H8OOH2-3                           1.000E+011     0.000
11750.0

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

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

!REF:GREEN 2003
C4H8OOH1-3=>OH+CH2O+C3H6                          6.635E+013    -0.160
29900.0
C4H8OOH2-4=>OH+CH3CHO+C2H4                        1.945E+018    -1.630
26790.0

!REF:ESTIMATE?
C4H8OOH1-2+O2<=>C4H8OOH1-2O2                      7.540E+012     0.000
0.0
C4H8OOH1-3+O2<=>C4H8OOH1-3O2                      7.540E+012     0.000
0.0
C4H8OOH1-4+O2<=>C4H8OOH1-4O2                      4.520E+012     0.000
0.0
C4H8OOH2-1+O2<=>C4H8OOH2-1O2                      4.520E+012     0.000
0.0
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C4H8OOH2-3+O2<=>C4H8OOH2-3O2                    7.540E+012     0.000
0.0
C4H8OOH2-4+O2<=>C4H8OOH2-4O2                    4.520E+012     0.000
0.0

!REF:
C4H8OOH1-2O2<=>NC4KET12+OH                      2.000E+011     0.000
31500.0
C4H8OOH1-3O2<=>NC4KET13+OH                      2.500E+010     0.000
21400.0
C4H8OOH1-4O2<=>NC4KET14+OH                      3.125E+009     0.000
19350.0
C4H8OOH2-1O2<=>NC4KET21+OH                      1.000E+011     0.000
28850.0
C4H8OOH2-3O2<=>NC4KET23+OH                      1.000E+011     0.000
28850.0
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
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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
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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
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!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<=>CH3CHOOCOCH3                       1.000E+011     0.000
0.0
CH3CHOOCOCH3<=>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                          1.200E+005     2.500
37560.0
NC3H7CHO+OH<=>NC3H7CO+H2O                          2.000E+006     1.800
-1300.0
NC3H7CHO+H<=>NC3H7CO+H2                            4.140E+009     1.120
2320.0
NC3H7CHO+O<=>NC3H7CO+OH                            5.940E+012     0.000
1868.0

!REF:HALF OF CH2O+HO2
NC3H7CHO+HO2<=>NC3H7CO+H2O2                        4.090E+004     2.500
10200.0

!REF:ANALOGY WITH ACETALDEHYDE
NC3H7CHO+CH3<=>NC3H7CO+CH4                         2.890E-003     4.620
3210.0
NC3H7CHO+CH3O<=>NC3H7CO+CH3OH                      1.000E+012     0.000
3300.0

!REF:PITZ ESTIMATE
NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H                    4.090E+004     2.500
10200.0

!REF:CURRAN ESTIMATE
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NC3H7CHO+OH<=>C3H6CHO-1+H2O                       5.280E+009     0.970
1586.0
NC3H7CHO+OH<=>C3H6CHO-2+H2O                       4.680E+007     1.610
-35.0
NC3H7CHO+OH<=>C3H6CHO-3+H2O                       5.520E+002     3.120
-1176.0
NC3H7CHO+HO2<=>C3H6CHO-1+H2O2                     2.379E+004     2.550
16490.0
NC3H7CHO+HO2<=>C3H6CHO-2+H2O2                     9.640E+003     2.600
13910.0
NC3H7CHO+HO2<=>C3H6CHO-3+H2O2                     3.440E+012     0.050
17880.0

!REF:CURRAN ESTIMATE
NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H                 2.379E+004     2.550
16490.0
NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H                 9.640E+003     2.600
13910.0
NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H                 3.440E+012     0.050
17880.0
NC3H7CO<=>NC3H7+CO                                1.000E+011     0.000
9600.0

!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95.
C3H6CHO-1<=>C2H4+CH2CHO                           7.400E+011     0.000
21970.0

!REF:CURRAN ESTIMATE
C2H5CHCO+H<=>C3H6CHO-3                            5.000E+012     0.000
1200.0
C2H3CHO+CH3<=>C3H6CHO-3                           1.230E+011     0.000
7800.0
!   CW70
!        reduce rate of sc3h5cho reaction
!SC3H5CHO+H<=>C3H6CHO-2                            5.000E+012     0.000
2900.0
SC3H5CHO+H<=>C3H6CHO-2                            1.000E+012     0.000
2900.0
!
C3H6+HCO<=>C3H6CHO-2                              1.000E+011     0.000
6000.0
C2H5CHCO+OH<=>NC3H7+CO2                           3.730E+012     0.000
-1010.0
C2H5CHCO+H<=>NC3H7+CO                             4.400E+012     0.000
1459.0
C2H5CHCO+O<=>C3H6+CO2                             3.200E+012     0.000
-437.0

!REF:ANALOGY WITH ACETALDEHYDE
!SC3H5CHO+OH<=>SC3H5CO+H2O                         2.690E+010     0.760
-340.0
!    CW70
!SC3H5CHO+OH<=>SC3H5CO+H2O                         2.690E+009     0.760
-340.0
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!    CW71
SC3H5CHO+OH<=>SC3H5CO+H2O                          2.690E+008     0.760
-340.0
!
!REF:PITZ ESTIMATE
C3H5-S+CO<=>SC3H5CO                                5.000E+012     0.000
8000.0

!REF:ANALOGY WITH IC3H5CHO+X --> IC3H5CO+HX
!SC3H5CHO+HO2<=>SC3H5CO+H2O2                        1.000E+012     0.000
11920.0
!SC3H5CHO+CH3<=>SC3H5CO+CH4                         3.980E+012     0.000
8700.0
!reduce rate of consumption of sc3h5cho
!SC3H5CHO+HO2<=>SC3H5CO+H2O2                        5.000E+011     0.000
11920.0
!SC3H5CHO+CH3<=>SC3H5CO+CH4                         2.000E+012     0.000
8700.0
!
SC3H5CHO+HO2<=>SC3H5CO+H2O2                        1.000E+011     0.000
11920.0
SC3H5CHO+CH3<=>SC3H5CO+CH4                         2.000E+011     0.000
8700.0
!
!SC3H5CHO+O<=>SC3H5CO+OH                            7.180E+012     0.000
1389.0
!SC3H5CHO+O2<=>SC3H5CO+HO2                          4.000E+013     0.000
37600.0
!SC3H5CHO+H<=>SC3H5CO+H2                            2.600E+012     0.000
2600.0
!
SC3H5CHO+O<=>SC3H5CO+OH                            1.000E+012     0.000
1389.0
SC3H5CHO+O2<=>SC3H5CO+HO2                          1.000E+013     0.000
37600.0
SC3H5CHO+H<=>SC3H5CO+H2                            2.600E+011     0.000
2600.0
!
!REF:CURRAN ESTIMATE
C2H3COCH3+OH<=>CH3CHO+CH3CO                        1.000E+011     0.000
0.0
C2H3COCH3+OH=>CH2CO+C2H3+H2O                       5.100E+011     0.000
1192.0
C2H3COCH3+HO2=>CH2CHO+CH3CO+OH                     6.030E+009     0.000
7949.0
C2H3COCH3+HO2=>CH2CO+C2H3+H2O2                     8.500E+012     0.000
20460.0
C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O                 3.970E+011     0.000
17050.0
C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H                 3.010E+012     0.000
17580.0

!REF:NEW FIT FROM TIBOR NAGY BASED ON:
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!REF:OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253
IC4H10(+M)<=>CH3+IC3H7(+M)                          2.520E+031    -4.102
91495.0
LOW/                                                2.410E+019     0.000
52576.0/
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                                    2.510E+098   -23.810
145300.0
IC4H10<=>IC4H9+H                                    9.850E+095   -23.110
147600.0

!REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)
IC4H10+H<=>TC4H9+H2                                 6.020E+005     2.400
2583.0
IC4H10+H<=>IC4H9+H2                                 1.810E+006     2.540
6756.0
IC4H10+CH3<=>TC4H9+CH4                              9.040E-001     3.460
4598.0
IC4H10+CH3<=>IC4H9+CH4                              1.360E+000     3.650
7154.0

!REF:JOE MICHAELS SYMP. PAPER 2008.
IC4H10+OH<=>TC4H9+H2O                               2.925E+004     2.531
-1659.0
IC4H10+OH<=>IC4H9+H2O                               6.654E+004     2.665
-168.9

!REF:ALLARA AND SHAW ANALOG
IC4H10+C2H5<=>IC4H9+C2H6                            1.510E+012     0.000
10400.0

!REF:FROM ISOBUTYL RATE
IC4H10+C2H5<=>TC4H9+C2H6                            1.000E+011     0.000
7900.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-
7054.
IC4H10+HO2<=>IC4H9+H2O2                             6.120E+001     3.590
17160.0

!REF: X0.666
IC4H10+HO2<=>TC4H9+H2O2                             4.332E+002     3.010
12090.0

!REF:FIT TO TSANG 90 AND COHEN DATA

!REF:NIST STANDARD REFERENCE DATABASE 17 -2Q98
IC4H10+O<=>TC4H9+OH                                 1.968E+005     2.402
1150.0
IC4H10+O<=>IC4H9+OH                                 4.046E+007     2.034
5136.0
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!REF:ANALOGY TO C3H8+CH3O
IC4H10+CH3O<=>IC4H9+CH3OH                          4.800E+011     0.000
7000.0

!REF:TAMURA ESTIMATE
IC4H10+CH3O<=>TC4H9+CH3OH                          1.900E+010     0.000
2800.0

!REF:
IC4H10+O2<=>IC4H9+HO2                              9.000E+013     0.000
52290.0
IC4H10+O2<=>TC4H9+HO2                              1.000E+013     0.000
48200.0

!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                        2.079E+000     3.970
18280.0

!REF:SCOTT AND WALKER C&F 129(4) 365--377 2002 (*1.5)
IC4H10+C2H5O2<=>IC4H9+C2H5O2H                      2.550E+013     0.000
20460.0

!REF:ANALOGY TO C2H6+HO2
IC4H10+CH3CO3<=>IC4H9+CH3CO3H                      2.550E+013     0.000
20460.0
IC4H10+NC3H7O2<=>IC4H9+NC3H7O2H                    2.550E+013     0.000
20460.0
IC4H10+IC3H7O2<=>IC4H9+IC3H7O2H                    2.550E+013     0.000
20460.0
IC4H10+IC4H9O2<=>IC4H9+IC4H9O2H                    2.550E+013     0.000
20460.0
IC4H10+TC4H9O2<=>IC4H9+TC4H9O2H                    2.550E+013     0.000
20460.0

!REF:ANALOGY WITH RH+RO2 --> R+RO2H
IC4H10+O2CHO<=>IC4H9+HO2CHO                        2.520E+013     0.000
20440.0
IC4H10+O2CHO<=>TC4H9+HO2CHO                        2.800E+012     0.000
16010.0

!REF:WESTBROOK ESTIMATE
IC4H10+SC4H9O2<=>IC4H9+SC4H9O2H                    2.250E+013     0.000
20460.0

!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE,
AUGUST, 1988
IC4H10+SC4H9O2<=>TC4H9+SC4H9O2H                    2.800E+012     0.000
16000.0

!REF:WESTBROOK ESTIMATE
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IC4H10+PC4H9O2<=>IC4H9+PC4H9O2H                    2.250E+013     0.000
20460.0

!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE,
AUGUST, 1988
IC4H10+PC4H9O2<=>TC4H9+PC4H9O2H                    2.800E+012     0.000
16000.0

!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                        1.366E+002     3.120
13190.0

!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE,
AUGUST, 1988
IC4H10+C2H5O2<=>TC4H9+C2H5O2H                      2.800E+012     0.000
16000.0
IC4H10+CH3CO3<=>TC4H9+CH3CO3H                      2.800E+012     0.000
16000.0
IC4H10+NC3H7O2<=>TC4H9+NC3H7O2H                    2.800E+012     0.000
16000.0
IC4H10+IC3H7O2<=>TC4H9+IC3H7O2H                    2.800E+012     0.000
16000.0
IC4H10+IC4H9O2<=>TC4H9+IC4H9O2H                    2.800E+012     0.000
16000.0
IC4H10+TC4H9O2<=>TC4H9+TC4H9O2H                    2.800E+012     0.000
16000.0

!REF:WESTBROOK AND PITZ ESTIMATE (1983)
IC4H10+IC4H9<=>TC4H9+IC4H10                        2.500E+010     0.000
7900.0

!REF:ESTIMATE
IC4H9+HO2<=>IC4H9O+OH                              7.000E+012     0.000
-1000.0
TC4H9+HO2<=>TC4H9O+OH                              7.000E+012     0.000
-1000.0
CH3O2+IC4H9<=>CH3O+IC4H9O                          7.000E+012     0.000
-1000.0
CH3O2+TC4H9<=>CH3O+TC4H9O                          7.000E+012     0.000
-1000.0

!REF:
IC4H9<=>TC4H9                                      3.560E+010     0.880
34600.0

!REF:CURRAN INT J CHEM KINET 38:250-275, 2006
!IC4H8+H<=>IC4H9                                   6.250E+011     0.510
2620.0
!C3H6+CH3<=>IC4H9                                  1.890E+003     2.670
6850.0
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!H+IC4H8<=>TC4H9                                  1.060E+012     0.510
1230.0

!REF:
TC4H9+O2<=>IC4H8+HO2                              8.370E-001     3.590
11960.0
IC4H9+O2<=>IC4H8+HO2                              1.070E+000     3.710
9322.0
NC3H7O2+IC4H9<=>NC3H7O+IC4H9O                     7.000E+012     0.000
-1000.0
NC3H7O2+TC4H9<=>NC3H7O+TC4H9O                     7.000E+012     0.000
-1000.0
NC3H7O2+IC4H7<=>NC3H7O+IC4H7O                     7.000E+012     0.000
-1000.0
SC4H9O2+IC4H9<=>SC4H9O+IC4H9O                     7.000E+012     0.000
-1000.0
SC4H9O2+TC4H9<=>SC4H9O+TC4H9O                     7.000E+012     0.000
-1000.0
PC4H9O2+IC4H9<=>PC4H9O+IC4H9O                     7.000E+012     0.000
-1000.0
PC4H9O2+TC4H9<=>PC4H9O+TC4H9O                     7.000E+012     0.000
-1000.0
PC4H9O2+IC4H7<=>PC4H9O+IC4H7O                     7.000E+012     0.000
-1000.0
SC4H9O2+IC4H7<=>SC4H9O+IC4H7O                     7.000E+012     0.000
-1000.0

!REF:
IC4H9+O2<=>IC4H9O2                                2.260E+012     0.000
0.0
!REF: F. Goldsmith JPCA, 2012
TC4H9+O2<=>TC4H9O2                                6.6946E+13   -0.3  -
187.2



!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION,
SEATTLE, AUGUST, 1988.
IC4H9O2+C4H10<=>IC4H9O2H+SC4H9                    1.120E+013     0.000
17700.0
TC4H9O2+C4H10<=>TC4H9O2H+SC4H9                    1.120E+013     0.000
17700.0

!REF:WESTBROOK ESTIMATE
IC4H9O2+C4H10<=>IC4H9O2H+PC4H9                    1.700E+013     0.000
20460.0
TC4H9O2+C4H10<=>TC4H9O2H+PC4H9                    1.700E+013     0.000
20460.0

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

!REF:ANALOGY TO C3H6+HO2.
IC4H9O2+C3H6<=>IC4H9O2H+C3H5-A                    5.350E-002     4.207
13288.1
TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A                    5.350E-002     4.207
13288.1

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

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

!REF:WESTBROOK ESTIMATE
TC4H9O2+CH4<=>TC4H9O2H+CH3                        1.130E+013     0.000
20460.0

!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986
H2+TC4H9O2<=>H+TC4H9O2H                           3.010E+013     0.000
26030.0
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!REF:WESTBROOK ESTIMATE
TC4H9O2+C2H6<=>TC4H9O2H+C2H5                    1.700E+013     0.000
20460.0
TC4H9O2+C3H8<=>TC4H9O2H+IC3H7                   2.000E+012     0.000
17000.0
TC4H9O2+C3H8<=>TC4H9O2H+NC3H7                   1.700E+013     0.000
20460.0
TC4H9O2+CH3OH<=>TC4H9O2H+CH2OH                  6.300E+012     0.000
19360.0
TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH               6.300E+012     0.000
19360.0
TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH               4.200E+012     0.000
15000.0

!REF:HALF OF CH2O+HO2
IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO                 2.800E+012     0.000
13600.0
TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO                 2.800E+012     0.000
13600.0
IC4H9O2+C2H3CHO<=>IC4H9O2H+C2H3CO               2.800E+012     0.000
13600.0
TC4H9O2+C2H3CHO<=>TC4H9O2H+C2H3CO               2.800E+012     0.000
13600.0
IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO               2.800E+012     0.000
13600.0
TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO               2.800E+012     0.000
13600.0

!REF:ESTIMATE?
IC4H9O2+HO2<=>IC4H9O2H+O2                       1.750E+010     0.000
-3275.0
TC4H9O2+HO2<=>TC4H9O2H+O2                       1.750E+010     0.000
-3275.0

!REF:WESTBROOK ESTIMATE
IC4H9O2+H2O2<=>IC4H9O2H+HO2                     2.400E+012     0.000
10000.0
TC4H9O2+H2O2<=>TC4H9O2H+HO2                     2.400E+012     0.000
10000.0
IC4H9O2+CH2O<=>IC4H9O2H+HCO                     1.300E+011     0.000
9000.0
TC4H9O2+CH2O<=>TC4H9O2H+HCO                     1.300E+011     0.000
9000.0

!REF:
IC4H9O2+CH3O2=>IC4H9O+CH3O+O2                   1.400E+016    -1.610
1860.0
TC4H9O2+CH3O2=>TC4H9O+CH3O+O2                   1.400E+016    -1.610
1860.0
IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2                 1.400E+016    -1.610
1860.0
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IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2                  1.400E+016    -1.610
1860.0
TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2                  1.400E+016    -1.610
1860.0
IC4H9O2+IC4H9O2=>O2+IC4H9O+IC4H9O                 1.400E+016    -1.610
1860.0
IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+TC4H9O2=>O2+TC4H9O+TC4H9O                 1.400E+016    -1.610
1860.0
IC4H9O2+PC4H9O2=>IC4H9O+PC4H9O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+PC4H9O2=>TC4H9O+PC4H9O+O2                 1.400E+016    -1.610
1860.0
IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2                 1.400E+016    -1.610
1860.0
IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2                 1.400E+016    -1.610
1860.0
IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2                 1.400E+016    -1.610
1860.0
TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2                 1.400E+016    -1.610
1860.0
IC4H9O2+HO2=>IC4H9O+OH+O2                         1.400E+016    -1.610
1860.0
TC4H9O2+HO2=>TC4H9O+OH+O2                         1.400E+016    -1.610
1860.0

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

!REF:PITZ ESTIMATE: ANALOGY WITH C2H4+CH3O2
IC4H9O2+C2H4<=>IC4H9O2H+C2H3                       8.590E+000     3.754
27132.0
!REF:WESTBROOK ESTIMATE
IC4H9O2+CH4<=>IC4H9O2H+CH3                         1.130E+013     0.000
20460.0

!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986
H2+IC4H9O2<=>H+IC4H9O2H                            3.010E+013     0.000
26030.0

!REF:WESTBROOK ESTIMATE
IC4H9O2+C2H6<=>IC4H9O2H+C2H5                       1.700E+013     0.000
20460.0
IC4H9O2+C3H8<=>IC4H9O2H+IC3H7                      2.000E+012     0.000
17000.0
IC4H9O2+C3H8<=>IC4H9O2H+NC3H7                      1.700E+013     0.000
20460.0
IC4H9O2+CH3OH<=>IC4H9O2H+CH2OH                     6.300E+012     0.000
19360.0
IC4H9O2+C2H5OH<=>IC4H9O2H+PC2H4OH                  6.300E+012     0.000
19360.0
IC4H9O2+C2H5OH<=>IC4H9O2H+SC2H4OH                  4.200E+012     0.000
15000.0

!REF:
IC4H9O2H<=>IC4H9O+OH                               1.500E+016     0.000
42500.0
TC4H9O2H<=>TC4H9O+OH                               5.950E+015     0.000
42540.0
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!REF:ANALOGY CH3O+X --> CH2O+HX TSANG/ HAMPSON 86
IC4H9O+HO2<=>IC3H7CHO+H2O2                          1.000E+012     0.000
0.0
IC4H9O+OH<=>IC3H7CHO+H2O                            1.810E+013     0.000
0.0
IC4H9O+CH3<=>IC3H7CHO+CH4                           2.400E+013     0.000
0.0
IC4H9O+O<=>IC3H7CHO+OH                              6.000E+012     0.000
0.0
IC4H9O+H<=>IC3H7CHO+H2                              1.990E+013     0.000
0.0

!REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006
IC3H7CHO+H<=>IC4H9O                                 1.000E+012     0.000
5860.0
CH2O+IC3H7<=>IC4H9O                                 5.000E+010     0.000
2330.0
CH3COCH3+CH3<=>TC4H9O                               1.500E+011     0.000
11900.0

!REF:!ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503 (1985).
IC4H9O+O2<=>IC3H7CHO+HO2                            1.930E+011     0.000
1660.0

!REF:PITZ ESTIMATE
TC4H9O+O2<=>IC4H8O+HO2                              8.100E+011     0.000
4700.0

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

!REF: X 2.0
IC4H8O<=>IC3H7CHO                                   4.180E+013     0.000
52720.0

!REF:
IC4H8O+OH<=>IC3H6CHO+H2O                            1.250E+012     0.000
0.0
IC4H8O+H<=>IC3H6CHO+H2                              1.250E+012     0.000
0.0
IC4H8O+HO2<=>IC3H6CHO+H2O2                          2.500E+012     0.000
15000.0
IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H                      2.500E+012     0.000
19000.0
IC4H8O+CH3<=>IC3H6CHO+CH4                           5.000E+010     0.000
10000.0
IC4H8O+O<=>IC3H6CHO+OH                              1.250E+012     0.000
0.0

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES
TC3H6CHO+H<=>IC3H7CHO                               2.000E+014     0.000
0.0

!REF:TSANG J. PHYS. CHEM. REF. DATA 17, 887 (1988)
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IC3H7+HCO<=>IC3H7CHO                                1.810E+013     0.000
0.0

!REF:
IC3H7CHO+HO2<=>IC3H7CO+H2O2                         3.000E+012     0.000
11920.0

!REF:BALDWIN, R.R.; WALKER, R.W.

!REF:SYMP. INTL. COMB. PROC. 1979, 17, 525.
IC3H7CHO+HO2<=>TC3H6CHO+H2O2                        8.000E+010     0.000
11920.0

!REF:BIRRELL, R.N.; TROTMAN-DICKENSON, A.F. J. CHEM. SOC. 1960, 2059
IC3H7CHO+CH3<=>IC3H7CO+CH4                          3.980E+012     0.000
8700.0

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

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

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

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

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

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

!REF:
IC4H8+OH<=>IC4H8OH                                  9.930E+011     0.000
-960.0
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IC4H8OH+O2<=>IO2C4H8OH                            1.200E+011     0.000
-1100.0
IO2C4H8OH=>CH3COCH3+CH2O+OH                       1.250E+010     0.000
18900.0
IC4H9O2<=>IC4H8O2H-I                              7.500E+010     0.000
24400.0
IC4H9O2<=>IC4H8O2H-T                              1.000E+011     0.000
29200.0
!TC4H9O2<=>IC4H8+HO2                               7.612E+042    -9.410
41490.0
!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-
5701
TC4H9O2<=>TC4H8O2H-I                              4.521E+009     1.200
33500.0

!REF:Goldsmith, JPCA, 2012
IC4H8O2H-I+O2<=>IC4H8OOH-IO2                      9.35316E+11  0.1   -
1010.88
IC4H8O2H-T+O2<=>IC4H8OOH-TO2                      5.04482E+12  -0.1  -
655.2
TC4H8O2H-I+O2<=>TC4H8OOH-IO2                      22844293817  0.5   -
786.24


!REF:
IC4H8OOH-IO2<=>IC4KETII+OH                        5.000E+010     0.000
21400.0
IC4H8OOH-TO2<=>IC4KETIT+OH                        4.000E+011     0.000
31500.0
!REF:ANALOGY TO 1ST ISOMERISATION
TC4H8OOH-IO2<=>TIC4H7Q2-I                         9.820E+007     1.300
21500.0
!REF:ANALOGY TO QOOH B-SCISSION
TIC4H7Q2-I<=>IC4H7OOH+HO2                         1.600E+012     0.230
15200.0
!!C4H8OOH2-4<=>C4H8O1-3+OH   032114ADD
!TIC4H7Q2-I=>TC4H7O2H-CYII+OH                      2.440E+009     0.780
18000.0
!!C4H8OOH2-4=>OH+CH3CHO+C2H4   032114ADD
!TC4H7O2H-CYII=>CH3COCH2+CH2O+OH                   3.080E+008     1.500
23500.0
!!NC4KET14=>CH2CH2CHO+CH2O+OH  032414ADD
!TIC4H7Q2-I=>TC3H5OOH+CH2O+OH                      1.500E+016     0.000
42000.0
!!PC4H9O2H<=>PC4H9O+OH  032414ADD
!TC3H5OOH=>CH3COCH2+OH                             1.500E+016     0.000
42500.0

!REF:CURRAN ESTIMATE
!IC4H7OOH+HO2<=>TIC4H7Q2-I                         1.000E+011     0.000
10600.0

!REF:
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IC4H8OOH-IO2<=>IIC4H7Q2-I                          3.750E+010     0.000
24400.0
IC4H8OOH-IO2<=>IIC4H7Q2-T                          1.000E+011     0.000
29200.0
IC4H8OOH-TO2<=>TIC4H7Q2-I                          6.000E+011     0.000
34500.0

!REF:CURRAN ESTIMATE
AC3H5OOH+CH2O2H<=>IIC4H7Q2-I                       8.500E+010     0.000
10600.0
IC4H7OOH+HO2<=>IIC4H7Q2-T                          1.000E+011     0.000
7800.0
CH2O2H<=>CH2O+OH                                   9.000E+014     0.000
1500.0
IC4KETII=>CH2O+C2H5CO+OH                           1.500E+016     0.000
42000.0
IC4KETIT=>CH3COCH3+HCO+OH                          9.500E+015     0.000
42540.0

!REF:
!IC4H8+HO2<=>TC4H8O2H-I                            3.970E+011     0.000
12620.0

!REF:GREEN 2003
IC4H8O2H-I<=>CC4H8O+OH                             4.470E+011     0.000
21900.0
IC4H8O2H-T<=>IC4H8O+OH                             3.090E+012     0.000
13400.0
!TC4H8O2H-I<=>IC4H8O+OH                            3.980E+012     0.000
17000.0

!REF:
IC4H8O2H-I=>OH+CH2O+C3H6                           8.451E+015    -0.680
29170.0


!CZ 27/01/2014
!!REF:LASKIN ET AL. IJCK 32 589-614 2000
!C3H5-T+CH3(+M)<=>IC4H8(+M)                        2.500E+013     0.000
0.0
!LOW/                                              4.270E+058   -11.940
9769.8/
!TROE/  1.750E-001  1.341E+003  6.000E+004  1.014E+004/
!IC4H7+H(+M)<=>IC4H8(+M)                           1.000E+014     0.000
0.0
!LOW/                                              6.650E+059   -12.000
5967.8/
!TROE/  2.000E-002  1.097E+003  1.097E+003  6.860E+003/
!H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/

IC4H8<=>IC4H7-I1+H                                 7.710E+069   -16.090
140000.0
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!REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H<=>IC4H9                                    1.000E+000     1.000
0.0
PLOG/      0.0013     7.990E+081   -23.161     22239.0/
PLOG/      0.0400     4.240E+068   -18.427     19665.0/
PLOG/      1.0000     1.040E+049   -11.500     15359.0/
PLOG/     10.0000     6.200E+041    -8.892     14637.0/
PLOG/    100.0000    -6.450E+031    -5.851      8177.8/
DUP
IC4H8+H<=>IC4H9                                    1.000E+000     1.000
0.0
PLOG/      0.0013     1.850E+026    -5.830      3865.8/
PLOG/      0.0400     2.820E+030    -6.490      5470.8/
PLOG/      1.0000     3.780E+028    -5.570      5625.1/
PLOG/     10.0000     1.460E+025    -4.280      5247.8/
PLOG/    100.0000     7.240E+026    -4.210      6825.0/
DUP
IC4H8+H<=>C3H6+CH3                                 1.000E+000     1.000
1.0
PLOG/      0.0013     1.540E+009     1.350      2542.0/
PLOG/      0.0400     7.880E+010     0.870      3599.6/
PLOG/      1.0000     2.670E+012     0.470      5431.1/
PLOG/     10.0000     9.250E+022    -2.600     12898.0/
PLOG/    100.0000     1.320E+023    -2.420     16500.0/
DUP
IC4H8+H<=>C3H6+CH3                                 1.000E+000     1.000
1.0
PLOG/     10.0000     1.240E+005     2.520      3679.1/
PLOG/    100.0000     2.510E+003     2.910      3980.9/
DUP
IC4H8+H<=>TC4H9                                    1.000E+000     1.000
1.0
PLOG/      0.0013     1.350E+044   -10.680      8196.4/
PLOG/      0.0400     2.110E+057   -14.230     15147.0/
PLOG/      1.0000     3.260E+061   -14.940     20161.0/
PLOG/     10.0000     5.300E+056   -13.120     20667.0/
PLOG/    100.0000     1.110E+050   -10.800     20202.0/
DUP
IC4H8+H<=>TC4H9                                    1.000E+000     1.000
1.0
PLOG/      0.0013     2.170E+130   -32.580    136140.0/
PLOG/      0.0400     2.250E+029    -5.840      4241.9/
PLOG/      1.0000     1.060E+030    -5.630      5613.4/
PLOG/     10.0000     6.110E+026    -4.440      5182.3/
PLOG/    100.0000     2.730E+023    -3.260      4597.0/
DUP
!C3H6+CH3<=>IC4H9                                  1.000E+000     1.000
1.0
!PLOG/      0.0013     8.670E+048   -12.540     18206.0/
!PLOG/      0.0400     1.060E+049   -12.040     20001.0/
!PLOG/      1.0000     7.670E+047   -11.170     22366.0/
!PLOG/     10.0000     1.810E+045   -10.030     23769.0/
!PLOG/    100.0000     2.040E+040    -8.250     24214.0/
!DUP
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!C3H6+CH3<=>IC4H9                                    1.000E+000     1.000
1.0
!PLOG/      0.0013     1.120E+043   -11.300     13080.0/
!PLOG/      0.0400     7.280E+039    -9.880     13164.0/
!PLOG/      1.0000     2.600E+033    -7.460     12416.0/
!PLOG/     10.0000     3.850E+027    -5.380     11455.0/
!PLOG/    100.0000     1.660E+021    -3.170     10241.0/
!DUP

! From K. Zhang estimated
IC4H9<=>C3H6+CH3 1.0 1.0 1.0
PLOG  / 1.000E-001 3.150E+041  -9.50  33486. / !FIT FROM: 500-2000 K
ERROR IN FIT: 34%
PLOG  / 1.000E+000 6.750E+044 -10.07  37209. / !FIT FROM: 500-2000 K
ERROR IN FIT: 29%
PLOG  / 1.000E+001 7.790E+044  -9.70  39751. / !FIT FROM: 500-2000 K
ERROR IN FIT: 19%
PLOG  / 1.000E+002 3.610E+039  -7.78  39583. / !FIT FROM: 500-2000 K
ERROR IN FIT: 10%

IC4H8+H<=>IC4H7+H2                                  7.29E+05     2.455
4361.2
IC4H8+H<=>IC4H7-I1+H2                               8.621E+02       3.25
        12166.98

!Ref: C ZHOU calculated at qcisd(t)/cbs//m062x/6-311++G(d,p) level of
theory
!IC4H8+OH<=>IC4H7+H2O                                43950.16898
     2.67841    -827.103
IC4H8+OH<=>IC4H7-I1+H2O                             5465.0474   2.81477
     1114.19989

! divided by 2 from the above
IC4H8+OH<=>IC4H7+H2O                                21975.08449 2.67841
     -827.103

IC4H8+OH<=>IC4H7OH+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/
IC4H8+OH<=>SC3H5OH+CH3                              1.290E+006     1.650
1233.0
PLOG/      0.0013     5.16E+05     1.650      1233.0/
PLOG/      0.0100     7.28E+03     2.100      1162.0/
PLOG/      0.0130     8.16E+02     2.480      1128.0/
PLOG/      0.0250     1.15E+02     2.800      1152.0/
PLOG/      0.1000     5.60E+00     3.210      1208.0/
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PLOG/      0.1315     3.08E+00     3.290      1216.0/
PLOG/      1.0000     4.52E+03     2.500      3238.0/
PLOG/     10.0000     9.64E+18    -1.740     13107.0/
PLOG/    100.0000     1.32E-01     3.700      3665.0/
IC4H8+OH<=>IC3H5OH+CH3                            1.290E+006     1.650
1233.0
PLOG/      0.0013     2.06E+06     1.650      1233.0/
PLOG/      0.0100     2.91E+04     2.100      1162.0/
PLOG/      0.0130     3.26E+03     2.480      1128.0/
PLOG/      0.0250     4.61E+02     2.800      1152.0/
PLOG/      0.1000     2.24E+01     3.210      1208.0/
PLOG/      0.1315     1.23E+01     3.290      1216.0/
PLOG/      1.0000     1.81E+04     2.500      3238.0/
PLOG/     10.0000     3.86E+19    -1.740     13107.0/
PLOG/    100.0000     5.28E-01     3.700      3665.0/
IC4H8+OH<=>SC4H7OH-I+H                                 2.870E+000     2.920
625.0
PLOG/      0.0013     2.870E+000     2.920       625.0/
PLOG/      0.0100     4.840E-001     2.980       704.0/
PLOG/      0.0130     3.130E-001     3.040       721.0/
PLOG/      0.0250     9.330E-003     3.620       677.0/
PLOG/      0.1000     4.640E-005     4.480       687.0/
PLOG/      0.1315     2.710E-005     4.560       707.0/
PLOG/      1.0000     7.650E-007     5.050       874.0/
PLOG/     10.0000     2.640E+015    -0.800     12728.0/
PLOG/    100.0000     4.870E-004     4.320      4020.0/
IC4H8+OH<=>CH3COCH3+CH3                                6.930E+005     1.490
-536.0
PLOG/      0.0013     6.930E+005     1.490      -536.0/
PLOG/      0.0100     5.940E+003     2.010      -560.0/
PLOG/      0.0130     1.100E+003     2.220      -680.0/
PLOG/      0.0250     1.070E+002     2.500      -759.0/
PLOG/      0.1000     7.830E-001     3.100      -919.0/
PLOG/      0.1315     3.070E-001     3.220      -946.0/
PLOG/      1.0000     3.160E-004     4.050     -1144.0/
PLOG/     10.0000     7.590E-006     4.490      -680.0/
PLOG/    100.0000     5.450E-005     4.220      1141.0/
IC4H8+OH<=>IC4H8OH1-2                                  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
IC4H8+OH<=>IC4H8OH1-2                                  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/
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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
IC4H8+OH<=>TC4H8OH-I                                  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
IC4H8+OH<=>TC4H8OH-I                                  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:ANALOGY WITH TSANG '92: C3H6+R<=>PRODUCTS
!IC4H8+H<=>IC4H7+H2                                   3.400E+005     2.500
2492.0

!REF: ANALOGY WITH C2H4
IC4H8+O<=>IC3H7+HCO                                  7.450E+006     1.880
183.0
IC4H8+O=>CH2CO+CH3+CH3                               3.050E+006     1.880
183.0
IC4H8+O=>IC3H6CO+H+H                                 3.050E+006     1.880
183.0
IC4H8+O<=>IC4H7+OH                                   1.05E+12       0.700
5884.0
IC4H8+O<=>IC4H7-I1+OH                                1.200E+011     0.700
8959.1

!REF: ORME J. P., CURRAN H. J., SIMMIE J. M. JPCA, 2006, 110, 114-131
!C3H4-A+CH3<=>IC4H7                                  1.89E+03      2.67
6850

! REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++g(d,p) LEVEL OF
THEORY
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C3H4-A+CH3<=>IC4H7                                  40209.73013  2.51815
8847.53569

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS
!IC4H8+O=>CH2CO+CH3+CH3                              3.330E+007     1.760
76.0

!REF:
!IC4H8+O=>IC3H6CO+H+H                                1.660E+007     1.760
76.0

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS
!IC4H8+O<=>IC4H7+OH                                  1.206E+011     0.700
7633.0

!REF: C-J CHEN AND J. W. BOZZELLI J. PHYS. CHEM. A, 2000, 104, 9715-9732.
!IC4H8+O2<=>IC4H7+HO2                                 1.86E+9        1.301
40939
IC4H8+O2<=>IC4H7-I1+HO2                              2.000E+013     0.000
62270.0

! multiply the above by 10
IC4H8+O2<=>IC4H7+HO2                                 1.86E+10        1.301
40939

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
IC4H8+CH3<=>IC4H7+CH4                                4.420E+000     3.500
5675.0
IC4H8+CH3<=>IC4H7-I1+CH4                             1.348E+000     3.500
12850.0

! REF:
IC4H8+HO2<=>IC4H9O2                                  1.085E+27     -5.2916
21883.0
IC4H8+HO2<=>IC4H8O2H-T                               3.970E+011     0.000
12620.0

!! REF: VILLANO, S, M.; CARSTENSEN, H-H.; DEAN, A. M. J. PHYS. CHEM. A.,
2013, 117, 6458.
!IC4H8+HO2<=>IC4H9O2                                  1.5E-1         3.41
11700
!IC4H8+HO2<=>IC4H8O2H-T                               1.64E4         2.43
8300

!REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
!IC4H8+HO2<=>IC4H7+H2O2                               2.92E-01    4.12
12802.0
!REF: C3 NUIG CALCULATION J.Mendes
IC4H8+HO2<=>IC4H7-I1+H2O2                            97038.94079   2.54892
24733.17153

!DIVIDED THE ABOVE BY A FACTOR OF 2
IC4H8+HO2<=>IC4H7+H2O2                               1.46E-01    4.12
12802.0
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!REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
IC4H8+HO2<=>TC4H9O2                                1.04E-01     3.45
4338.0
IC4H8+HO2<=>TC4H8O2H-I                             1.000E+011     0.000
0.0
PLOG/    0.013   6.67E+14    -2.14 14188/
PLOG/    0.9869  6.25E+06    0.64  9073 /
PLOG/    9.869   7.96E+06    0.82  8771 /
PLOG/    98.69   2.05E+13    -0.82 12919/
IC4H8+HO2<=>IC4H8O+OH                             1.000E+011     0.000
0.0
PLOG/    0.013   1.18E+04    2.29  11321/
PLOG/    0.9869  5.30E+04    2.10  11797/
PLOG/    9.869   1.47E+09    0.83  14808/
PLOG/    98.69   1.96E+17    -1.45 21195/
TC4H8O2H-I<=>IC4H8O+OH                             1.000E+011     0.000
0.0
PLOG/    0.013   5.23E+17    -2.97 8215/
PLOG/    0.9869  4.39E+22    -3.90    11424/
PLOG/    9.869   4.00E+25    -4.50    13952/
PLOG/    98.69   1.21E+27    -4.66    16324/

!REF: ANOLOGY WITH C3H5-A+HO2
IC4H7+CH3O2<=>IC4H7O+CH3O                          1.000E+011     0.000
0.0
PLOG/      0.0100     2.31E+12  -0.11319 -1530.82661/
PLOG/      0.1000     9.81E+10  0.26264  -2724.0257/
PLOG/      1.0000     1.08E+10  0.5209   -3703.7221/
PLOG/     10.0000     8.92E+08  0.85906  -4676.45336/
PLOG/    100.0000     1.83E+09  0.85551  -4184.92838/

!REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325-3346
IC4H7+HO2<=>IC4H7O+OH                              1.000E+011     0.000
0.0
PLOG/      0.0100     1.020E+013    -0.158     -1417.0/
PLOG/      0.1000     4.980E+014    -0.642      -349.1/
PLOG/      1.0000     7.770E+017    -1.520      2379.2/
PLOG/     10.0000     2.930E+015    -0.684      3615.3/
PLOG/    100.0000     1.640E+004     2.740      1144.4/
IC4H7+HO2<=>IC4H7OOH                               1.000E+011     0.000
0.0
PLOG/      0.0100     1.910E+031    -7.230      1336.2/
PLOG/      0.1000     6.310E+042   -10.300      5568.9/
PLOG/      1.0000     1.030E+045   -10.600      7851.5/
PLOG/     10.0000     2.790E+037    -7.920      6497.9/
PLOG/    100.0000     1.440E+032    -6.010      6053.6/
IC4H7+HO2<=>IC3H5CHO+H2O                           1.000E+011     0.000
0.0
PLOG/      0.0100     1.090E+000     3.010     -3421.1/
PLOG/      0.1000     6.350E+001     2.500     -2341.4/
PLOG/      1.0000     6.050E+005     1.390       595.1/
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PLOG/     10.0000     3.100E+005     1.590      2677.6/
PLOG/    100.0000     5.070E-005     4.590       927.5/
IC4H7OOH<=>IC3H5CHO+H2O                              1.000E+011     0.000
0.0
PLOG/      0.0100     1.990E+050   -12.700     53531.9/
PLOG/      0.1000     4.720E+047   -11.500     54360.9/
PLOG/      1.0000     1.500E+040    -8.840     53179.2/
PLOG/     10.0000     2.540E+028    -5.000     49919.4/
PLOG/    100.0000     1.480E+016    -1.120     45949.3/
IC4H7OOH<=>IC4H7O+OH                                 1.000E+011     0.000
0.0
PLOG/      0.0100     1.490E+058   -13.900     54266.9/
PLOG/      0.1000     1.800E+054   -12.400     54193.8/
PLOG/      1.0000     3.360E+046    -9.810     52468.5/
PLOG/     10.0000     2.390E+036    -6.540     49429.0/
PLOG/    100.0000     1.280E+027    -3.610     46333.1/
IC4H7O<=>C3H5-T+CH2O                                 1.000E+011     0.000
0.0
PLOG/      0.0010     7.260E+006     0.182     17815.5/
PLOG/      0.0100     6.970E+016    -2.500     20878.7/
PLOG/      0.1000     6.640E+023    -4.230     23565.0/
PLOG/      1.0000     1.070E+026    -4.560     24622.9/
PLOG/     10.0000     6.500E+029    -5.370     26645.0/
PLOG/    100.0000     4.630E+031    -5.590     28915.3/
PLOG/   1000.0000     8.520E+025    -3.610     27863.4/
IC4H7O<=>IC3H5OCH2                                   1.000E+011     0.000
0.0
PLOG/      0.0010     3.170E+020    -4.150     12121.3/
PLOG/      0.0100     4.790E+024    -5.030     14606.1/
PLOG/      0.1000     1.900E+026    -5.160     16124.4/
PLOG/      1.0000     1.510E+028    -5.400     18165.4/
PLOG/     10.0000     2.420E+028    -5.170     19691.2/
PLOG/    100.0000     5.570E+024    -3.860     19395.2/
PLOG/   1000.0000     1.350E+018    -1.730     17386.5/
IC4H7O<=>IC3H6CHO                                    1.000E+011     0.000
0.0
PLOG/      0.0010     5.250E-049    15.500    -15639.9/
PLOG/      0.0100     1.460E-088    27.600    -35995.0/
PLOG/      0.1000     4.440E-022     8.380     -3819.0/
PLOG/      1.0000     6.230E+012    -1.440     10829.2/
PLOG/     10.0000     3.480E+042    -9.910     25297.9/
PLOG/    100.0000     1.880E+038    -8.160     25974.5/
PLOG/   1000.0000     1.670E+021    -2.740     20337.7/
IC4H7O<=>IC3H5CHO+H                                  1.000E+011     0.000
0.0
PLOG/      0.0010     3.000E+015    -2.310     14667.9/
PLOG/      0.0100     1.500E+022    -3.960     18283.0/
PLOG/      0.1000     1.950E+023    -3.990     19143.3/
PLOG/      1.0000     1.150E+025    -4.240     20311.2/
PLOG/     10.0000     1.760E+028    -4.890     22765.2/
PLOG/    100.0000     1.410E+027    -4.280     23770.6/
PLOG/   1000.0000     2.570E+020    -2.060     22040.1/
IC4H7O<=>C3H6+HCO                                    1.000E+011     0.000
0.0
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PLOG/      0.0010     6.620E+016    -2.840     13197.0/
PLOG/      0.0100     1.260E+020    -3.530     15469.2/
PLOG/      0.1000     2.130E+021    -3.640     16584.5/
PLOG/      1.0000     1.070E+024    -4.160     18985.0/
PLOG/     10.0000     8.420E+025    -4.400     22382.6/
PLOG/    100.0000     1.860E+021    -2.730     23658.8/
PLOG/   1000.0000     4.750E+008     1.140     20922.5/
IC3H5OCH2<=>C3H5-T+CH2O                              1.000E+011     0.000
0.0
PLOG/      0.0010     3.300E+009    -0.638     19747.8/
PLOG/      0.0100     3.360E+021    -3.900     23945.2/
PLOG/      0.1000     2.910E+029    -5.900     27249.7/
PLOG/      1.0000     1.830E+034    -6.940     30690.4/
PLOG/     10.0000     9.720E+033    -6.500     33002.5/
PLOG/    100.0000     2.680E+027    -4.260     33305.6/
PLOG/   1000.0000     8.810E+014    -0.326     31553.1/
IC3H5OCH2<=>IC3H6CHO                                 1.000E+011     0.000
0.0
PLOG/      0.0010     8.010E-092    27.800    -37321.2/
PLOG/      0.0100     7.780E-011     3.700     -2766.9/
PLOG/      0.1000     5.110E+015    -2.760     15937.6/
PLOG/      1.0000     4.480E+025    -5.200     21532.2/
PLOG/     10.0000     3.970E+034    -7.410     28116.9/
PLOG/    100.0000     5.620E+022    -3.560     25806.7/
PLOG/   1000.0000     2.510E+020    -2.630     29288.4/
IC3H5OCH2<=>IC3H5CHO+H                               1.000E+011     0.000
0.0
PLOG/      0.0010     4.930E+024    -5.050     20108.4/
PLOG/      0.0100     2.140E+028    -5.800     22219.4/
PLOG/      0.1000     1.930E+032    -6.640     25108.2/
PLOG/      1.0000     8.600E+034    -7.110     28209.1/
PLOG/     10.0000     2.170E+034    -6.640     30647.6/
PLOG/    100.0000     4.170E+028    -4.710     31231.9/
PLOG/   1000.0000     3.980E+018    -1.620     30129.8/
IC3H5OCH2<=>C3H6+HCO                                 1.000E+011     0.000
0.0
PLOG/      0.0010     8.230E+026    -5.840     19356.9/
PLOG/      0.0100     1.320E+029    -6.210     21293.6/
PLOG/      0.1000     3.470E+032    -6.960     24197.3/
PLOG/      1.0000     1.440E+036    -7.760     28007.8/
PLOG/     10.0000     9.720E+037    -8.020     32394.6/
PLOG/    100.0000     2.430E+031    -5.810     34295.8/
PLOG/   1000.0000     3.730E+014    -0.726     32008.3/
IC3H6CHO<=>C3H5-T+CH2O                               1.000E+011     0.000
0.0
PLOG/      0.0010     6.890E-069    21.500      2638.0/
PLOG/      0.0100     5.340E-033    11.100     16749.1/
PLOG/      0.1000     6.110E+026    -6.010     44116.7/
PLOG/      1.0000     8.040E+035    -8.310     46919.7/
PLOG/     10.0000     5.520E+040    -9.190     50508.7/
PLOG/    100.0000     5.850E+035    -7.180     52038.4/
PLOG/   1000.0000     1.930E+019    -1.940     48440.0/
IC3H6CHO<=>IC3H5CHO+H                                1.000E+011     0.000
0.0
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PLOG/      0.0010     1.610E+010    -1.240     32371.3/
PLOG/      0.0100     5.840E+015    -2.610     32878.4/
PLOG/      0.1000     3.640E+023    -4.600     34275.3/
PLOG/      1.0000     7.580E+031    -6.630     37895.4/
PLOG/     10.0000     2.860E+032    -6.300     39990.7/
PLOG/    100.0000     1.570E+023    -3.140     38011.7/
PLOG/   1000.0000     4.520E+012     0.214     34570.5/
IC3H6CHO<=>C3H6+HCO                                  1.000E+011     0.000
0.0
PLOG/      0.0010     2.900E+032    -7.240     25687.5/
PLOG/      0.0100     5.300E+033    -7.280     27100.6/
PLOG/      0.1000     2.000E+035    -7.410     29027.3/
PLOG/      1.0000     1.010E+034    -6.700     30018.1/
PLOG/     10.0000     9.760E+027    -4.630     28923.9/
PLOG/    100.0000     2.110E+019    -1.850     26239.8/
PLOG/   1000.0000     1.590E+013     0.063     24086.3/
C3H5-T+CH2O<=>IC3H5CHO+H                             1.000E+011     0.000
0.0
PLOG/      0.0010     2.600E+004     2.260      1510.3/
PLOG/      0.0100     5.130E+004     2.170      1675.5/
PLOG/      0.1000     3.990E+005     1.910      2218.3/
PLOG/      1.0000     1.750E+007     1.450      3428.0/
PLOG/     10.0000     1.350E+009     0.933      5173.0/
PLOG/    100.0000     2.240E+011     0.357      8001.3/
PLOG/   1000.0000     6.010E+005     2.090      7895.6/
C3H5-T+CH2O<=>C3H6+HCO                               1.000E+011     0.000
0.0
PLOG/      0.0010     1.110E+007     1.090      1807.2/
PLOG/      0.0100     2.470E+007     0.993      1994.9/
PLOG/      0.1000     2.470E+008     0.704      2596.2/
PLOG/      1.0000     1.420E+010     0.209      3934.2/
PLOG/     10.0000     3.450E+013    -0.726      6944.3/
PLOG/    100.0000     3.310E+014    -0.866     10965.7/
PLOG/   1000.0000     1.650E+001     3.170      9399.8/

!REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104,
9715-9732.
! HIGH PRESSURE LIMIT ONLY
IC4H7+O2<=>IC4H7O2                                   1.09E+010     0.56725
2290
IC4H7O2<=>IC4H7O+O                                   1.82E+014     0.0
60620
IC4H7O2<=>IC3H5CHO+OH                                1.52E+009     1.02524
39460
IC4H7O2<=>IC4H6OOH-I                                 1.41E+005     1.83586
19820
IC4H6OOH-I<=>C*CYCCOC+OH                             6.82E+012    -0.34545
42140
IC4H6OOH-I<=>C3H4-A+CH2O2H                           1.18E+012     0.91203
51390
IC4H6OOH-I<=>IC3H5CHO+OH                             2.42E+009     0.87390
54090
IC4H7O2<=>CCYCCOOC-T1                                1.19E+008     0.80412
28020
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CCYCCOOC-T1<=>CCYCCOOC-I2                          3.56E+013     0.0
38820
CCYCCOOC-I2<=>CHOIC3H6O                           3.19E+014     0.0
3000
CHOIC3H6O<=>CH3CHCHO+CH2O                         4.30E+012     0.0
9780
CCYCCOOC-T1<=>CCY(C2O)CO                          4.56E+011     0.92729
17470
CCY(C2O)CO<=>CCYCCO-T1+CH2O                       1.74E+013     0.0
18150
!IC4H7O2<=>C2CYCOOC-I1                             1.07E+008     0.89161
29720
C2CYCOOC-I1<=>IC3H5OOCH2                          4.41E+013    -0.22618
18500
IC3H5OOCH2<=>CH3COCH2+CH2O                        1.41E+010     0.0
1000
C2CYCOOC-I1<=>CCY(C2O)CO                          1.21E+013     0.10180
20320

!IC4H6OOH-I+O2<=>O2IC4H6OOH-I                      1.09E+010     0.56725
2290
!O2IC4H6OOH-I<=>HO2IC3H4CHO                       4.00E+010     0.0
18580
!HO2IC3H4CHO<=>OIC3H4CHO+OH                       2.00E+016     0.0
40500

!REF: LILI YE AND STEPHEN J KLIP[PENSTEIN PROCEEDING OF COMBUSTION
INSTITUTE, 2014
!BASED ON C3H6 THERMO DECOMPOSITION

CH2+C3H6<=>CCYCCC                                  1.000E+011     0.000
0.0
PLOG/      0.0100     1.44E+51    -13.12     14153/
PLOG/      0.1000     3.38E+54    -13.55     16473/
PLOG/      1.0000     1.35E+54    -12.97     18862/
PLOG/     10.0000     2.73E+47    -10.78     14232/
PLOG/    100.0000     2.71E+50    -11.22     16720/
DUP
CH2+C3H6<=>CCYCCC                                  1.000E+011     0.000
0.0
PLOG/      0.0100     6.16E+40    -10.5 5428.1/
PLOG/      0.1000     6.93E+41    -10.3 6188.9/
PLOG/      1.0000     1.81E+37    -8.55 5521/
PLOG/     10.0000     4.26E+37    -8.32 4770.2/
PLOG/    100.0000     4.68E+35    -7.37 4689.1/
DUP

CH2+C3H6<=>IC4H8                                   1.000E+011     0.000
0.0
PLOG/      0.0100     4.82E+57    -14.34     17091/
PLOG/      0.1000     3.84E+59    -14.36     18427/
PLOG/      1.0000     2.13E+58    -13.45     20355/
PLOG/     10.0000     8.48E+52    -11.63     20677/
PLOG/    100.0000     6.07E+47    -9.85 22055/
```

```
DUP
CH2+C3H6<=>IC4H8                                  1.000E+011     0.000
0.0
PLOG/      0.0100     1.15E+45    -11.13      6145.2/
PLOG/      0.1000     1.83E+45    -10.68      6638.5/
PLOG/      1.0000     1.30E+40    -8.7703     5863.8/
PLOG/     10.0000     2.27E+32    -6.1375     4317.9/
PLOG/    100.0000     1.28E+24    -3.4904     2529.9/
DUP

CH2+C3H6<=>IC4H7+H                                 1.000E+011     0.000
0.0
PLOG/      0.0100     8.20E+19    -2.06 1145.2/
PLOG/      0.1000     2.27E+21    -2.44 2648.4/
PLOG/      1.0000     4.44E+35    -6.55 13894/
PLOG/     10.0000     1.18E+28    -4.09 14013/
PLOG/    100.0000     6.51E+26    -3.58 18927/
DUP
CH2+C3H6<=>IC4H7+H                                 1.000E+011     0.000
0.0
PLOG/      0.0100     1.08E+07    1.62  -3174.6/
PLOG/      0.1000     1.37E+05    2.15  -3799.2/
PLOG/      1.0000     3.89E+14    -0.42 1237.6/
PLOG/     10.0000     2.45E+10    0.67  750.93/
PLOG/    100.0000     1.81E+02    2.97  -746.03/
DUP

CH2+C3H6<=>C3H5-T+CH3                                 1.000E+011     0.000
0.0
PLOG/      0.0100     1.77E+19    -1.94 6786.8/
PLOG/      0.1000     1.68E+19    -1.8  4310.4/
PLOG/      1.0000     4.16E+24    -3.19 9758.5/
PLOG/     10.0000     7.89E+24    -3.07 13894/
PLOG/    100.0000     7.36E+29    -4.28 23849/
DUP
CH2+C3H6<=>C3H5-T+CH3                              1.000E+011     0.000
0.0
PLOG/      0.0100     4.30E+12    0.19  -110.41/
PLOG/      0.1000     2.26E+11    0.54  47.81/
PLOG/      1.0000     4.92E+09    1.02  599.77/
PLOG/     10.0000     1.47E+08    1.33  1228.4/
PLOG/    100.0000     8.11E+10    0.55  5506.5/
DUP

C3H5-T+CH3<=>IC4H8                                 1.000E+011     0.000
0.0
PLOG/      0.0100     1.93E+61    -14.91      19559/
PLOG/      0.1000     7.49E+58    -13.81      20442/
PLOG/      1.0000     9.74E+55    -12.62      21930/
PLOG/     10.0000     7.70E+50    -10.88      22198/
PLOG/    100.0000     2.07E+48    -9.9  24315/
DUP
C3H5-T+CH3<=>IC4H8                                 1.000E+011     0.000
0.0
```

```
PLOG/      0.0100     3.78E+46    -11.15     7331.5/
PLOG/      0.1000     2.86E+40    -8.97 6234.4/
PLOG/      1.0000     7.24E+33    -6.71 4848.4/
PLOG/     10.0000     2.28E+27    -4.53 3329.3/
PLOG/    100.0000     5.40E+23    -3.31 2521.8/
DUP

C3H5-T+CH3<=>IC4H7+H                              1.000E+011     0.000
0.0
PLOG/      0.0100     4.12E+29    -4.95 7995.8/
PLOG/      0.1000     4.86E+30    -5.03 11287/
PLOG/      1.0000     5.30E+29    -4.57 14443/
PLOG/     10.0000     1.32E+30    -4.54 19255/
PLOG/    100.0000     5.16E+28    -4.03 23821/
DUP
C3H5-T+CH3<=>IC4H7+H                              1.000E+011     0.000
0.0
PLOG/      0.0100     5.73E+15    -0.77 1195.9/
PLOG/      0.1000     2.06E+13    -0.074     1428.7/
PLOG/      1.0000     4.48E+10    0.6       1421.6/
PLOG/     10.0000     4.10E+06    1.71  1056.9/
PLOG/    100.0000     1.37E-01    3.91  -353.55/
DUP

IC4H7+H<=>IC4H8                                  1.000E+011     0.000
0.0
PLOG/      0.0100     2.00E+64    -15.02     23890/
PLOG/      0.1000     1.40E+61    -13.84     24846/
PLOG/      1.0000     1.00E+58    -12.7 25947 /
PLOG/     10.0000     1.68E+53    -11.13     25910/
PLOG/    100.0000     6.89E+44    -8.62 22842 /
DUP
IC4H7+H<=>IC4H8                                  1.000E+011     0.000
0.0
PLOG/      0.0100     1.85E+40    -8.58 6466.1/
PLOG/      0.1000     3.37E+34    -6.64 5193/
PLOG/      1.0000     9.06E+29    -5.1  4171.5/
PLOG/     10.0000     4.77E+25    -3.68 3143.1/
PLOG/    100.0000     1.10E+21    -2.16 1916.5/
DUP

IC4H8<=>CCYCCC                                  1.000E+011     0.000       0.0
PLOG/      0.0100     1.26E+64    -15.57     95033/
PLOG/      0.1000     3.94E+67    -16.19     100780/
PLOG/      1.0000     6.14E+68    -16.15     105890/
PLOG/     10.0000     9.70E+66    -15.301    109000/
PLOG/    100.0000     1.45E+62    -13.64     110210/
DUP
IC4H8<=>CCYCCC                                  1.000E+011     0.000       0.0
PLOG/      0.0100     4.84E+41    -9.62 79528/
PLOG/      0.1000     8.07E+44    -10.21     82671/
PLOG/      1.0000     1.15E+47    -10.56     85502/
PLOG/     10.0000     1.33E+39    -7.98 83303/
PLOG/    100.0000     4.97E+31    -5.6  80987/
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DUP

CCYCCC<=>IC4H7+H                                1.000E+011     0.000
0.0
PLOG/      0.0100     2.33E+63    -14.55      103320/
PLOG/      0.1000     7.03E+63    -14.37      107160/
PLOG/      1.0000     5.07E+64    -14.29      112340/
PLOG/     10.0000     4.92E+61    -13.15      114870/
PLOG/    100.0000     4.82E+57    -11.73      118250/
DUP
CCYCCC<=>IC4H7+H                                1.000E+011     0.000
0.0
PLOG/      0.0100     1.12E+40    -8.37 85836/
PLOG/      0.1000     1.06E+41    -8.33 88499/
PLOG/      1.0000     8.23E+43    -8.88 92907/
PLOG/     10.0000     1.27E+39    -7.33 93401/
PLOG/    100.0000     1.45E+28    -4.02 90995/
DUP

CCYCCC<=>C3H5-T+CH3                               1.000E+011     0.000
0.0
PLOG/      0.0100     8.31E+64    -15.14      111300/
PLOG/      0.1000     8.29E+64    -14.72      113700/
PLOG/      1.0000     1.00E+70    -15.72      121940/
PLOG/     10.0000     1.66E+67    -14.59      124380/
PLOG/    100.0000     7.87E+62    -13.05      126800/
DUP
CCYCCC<=>C3H5-T+CH3                             1.000E+011     0.000
0.0
PLOG/      0.0100     1.51E+49    -11.04      99748/
PLOG/      0.1000     1.05E+45    -9.46 99275/
PLOG/      1.0000     3.39E+50    -10.63      104220/
PLOG/     10.0000     1.76E+47    -9.43 104930/
PLOG/    100.0000     1.88E+39    -6.93 103980/
DUP

!ANALOGY WITH C3H5-A+CH3
IC4H7+CH3(+M)<=>AC5H10(+M)                       1.000E+014    -0.320
-262.3
LOW/                                              3.910E+060   -12.810
6250.0/
TROE/  1.040E-001  1.606E+003  6.000E+004  6.118E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/

!!REF:  FRIDLYAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4750-4761
!IC4H7+IC4H7<=>H15DE25DM                          1.000E+011     0.000
0.0
!PLOG/     0.039     6.54954E+64    -15.935     20230/
!PLOG/     0.078     1.50041E+60    -14.49      18600/
!PLOG/     0.156     2.27097E+55    -12.995     16700/
IC4H7+IC4H7<=>C3H4-A+AC5H10                                  9.550E+040
-9.300   12470.0
plog/      1.0000     4.10E+40    -9.300     12470.0/
```

```
plog/      4.0000     3.41E+32    -6.800      9180.0/
plog/     10.0000     1.26E+28    -5.500      7410.0/

! devided by 2 of the above
IC4H7+IC4H7<=>H15DE25DM                              1.000E+011     0.000
0.0
PLOG/     0.039     3.27E+64    -15.935     20230/
PLOG/     0.078     7.50E+59    -14.49      18600/
PLOG/     0.156     1.14E+55    -12.995     16700/

!H15DE25DM+OH=>C3H5-T+B13DE2M+H2O                                  1.79E+05
      2.636965672 -6.0
!H15DE25DM+OH=>C3H4-A+C2H4+C3H5-T+H2O                              5.064E+05
         2.46     729.44

!REF: FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+OH<=>AC5H9-A2+H2O                                           3.120E+06
      2.000 -298.0
AC5H10+H<=>AC5H9-A2+H2                                             1.730E+05
      2.500 2492.0
AC5H10+CH3<=>AC5H9-A2+CH4                                          2.210E+00
      3.500 5675.0
AC5H10+O<=>AC5H9-A2+OH                                             3.700E+05
2.56   -1.130E+03
AC5H10+OH<=>SC4H9+CH2O                                             2.000E+10
      0.000 4000.0
AC5H10+O<=>SC4H9+HCO                                               7.230E+05
      2.340 -1050.0
AC5H10+O<=>IC3H7+CH3CO                                             7.230E+05
      2.340 -1050.0
AC5H10+O<=>IC4H9+HCO                                              7.230E+05
      2.340 -1050.0
AC5H10<=>C3H5-T+C2H5                                               8.922E+24
      -2.409     100500.0
AC5H9-A2<=>C3H4-A+C2H5                                             1.983E+20 -
1.63   5.924E+04

!ref:-S is estimated
H15DE25DM+H<=>H15DE25DM-S+H2                                      1.42E+06
      2.315165407 2075.955844
H15DE25DM+H<=>H15DE25DM-A+H2                                      7.29E+05
2.455    4361.2

!H15DE25DM+OH<=>H15DE25DM-S+H2O                                    1.79E+05
      2.636965672 -6.0
!H15DE25DM+OH<=>H15DE25DM-A+H2O                                    5.064E+05
2.46     729.44

H15DE25DM+HO2<=>H15DE25DM-S+H2O2                                  1.00E+00
      3.887366896 9386.357213
H15DE25DM+HO2<=>H15DE25DM-A+H2O2                                   2.92E-01
4.12   12802.0
```

```
H15DE25DM+CH3<=>H15DE25DM-S+CH4                          1.00E+00
      3.649020008 3374.05195
H15DE25DM+CH3<=>H15DE25DM-A+CH4                           4.420E+000
3.500    5675.0

H15DE25DM+O2<=>H15DE25DM-S+HO2                           4.000E+014
0.000   38890.0
H15DE25DM+O2<=>H15DE25DM-A+HO2                           1.86E+9
1.301   40939

H15DE25DM+O<=>H15DE25DM-S+OH                             1.59243E+11
       0.7      1.30E+01
H15DE25DM+O<=>H15DE25DM-A+OH                             1.05E+12
0.700    5884.0

! DIVIDED BY A FACTOR OF 2 FROM THE ABOVE
H15DE25DM+OH<=>H15DE25DM-S+H2O                           8.95E+04
      2.636965672 -6.0
H15DE25DM+OH<=>H15DE25DM-A+H2O                           2.53E+05
2.46     729.44


!!ref:-S is estimated *100
!H15DE25DM+H<=>H15DE25DM-S+H2                            1.42E+08
      2.315165407 2075.955844
!H15DE25DM+H<=>H15DE25DM-A+H2                            7.29E+07
2.455    4361.2
!
!H15DE25DM+OH<=>H15DE25DM-S+H2O                          1.79E+07
      2.636965672 -6.0
!H15DE25DM+OH<=>H15DE25DM-A+H2O                          5.064E+07
2.46     729.44
!
!H15DE25DM+HO2<=>H15DE25DM-S+H2O2                        1.00E+02
      3.887366896 9386.357213
!H15DE25DM+HO2<=>H15DE25DM-A+H2O2                         2.92E+01
4.12   12802.0
!
!H15DE25DM+CH3<=>H15DE25DM-S+CH4                         1.00E+02
      3.649020008 3374.05195
!H15DE25DM+CH3<=>H15DE25DM-A+CH4                          4.420E+02
3.500    5675.0
!
!H15DE25DM+O2<=>H15DE25DM-S+HO2                          4.000E+016
0.000   38890.0
!H15DE25DM+O2<=>H15DE25DM-A+HO2                          1.86E+11
1.301   40939
!
!H15DE25DM+O<=>H15DE25DM-S+OH                            1.59243E+13
       0.7      1.30E+01
!H15DE25DM+O<=>H15DE25DM-A+OH                            1.05E+14
0.700    5884.0

! C ZHOU ESTIMATED
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!H15DE25DM-S<=>C3H5-T+B13DE2M                              3.501E+10
1.4677      50933.1
C3H4-A+B1E2M4J<=>H15DE25DM-A                             8.80E+03       2.48
6130

! MULTIPLY THE ABOVE BY 2
H15DE25DM-S<=>C3H5-T+B13DE2M                               7.002E+10
1.4677      50933.1

C2H3+C3H5-T<=>B13DE2M                                    8E+12 0.0 0.0
H+B13DE2MJ<=>B13DE2M                                    1E+14 0.0 0.0

!! ABSTRACTIONS FROM ALLYLIC -CH3 ANALOGY TO PROPENE

B13DE2M+HO2  <=> B13DE2MJ+H2O2        2.700E+004 2.500   12340.0
B13DE2M+H    <=> B13DE2MJ+H2          1.730E+005 2.500    2492.0
B13DE2M+O2   <=> B13DE2MJ+HO2         4.000E+012 0.000   39900.0
B13DE2M+CH3  <=> B13DE2MJ+CH4         2.210E+000 3.500    5675.0
B13DE2M+CH3O2<=> B13DE2MJ+CH3O2H      3.240E+011 0.000   14900.0
B13DE2M+OH   <=> B13DE2MJ+H2O         1.970E+006 2.200     540.0

C2H3+C3H4-A  <=>B13DE2MJ 9.45E+02  2.67 6850
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!! HYDROGEN ATOM ADDITIONS AND HO2 OXIDATIONS OF ALLYLIC SITES

B13DE2M+H       <=> B1E2M4J         2.50E+11  0.51   2620
!<INTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
(4) (2006) 250-275.
C2H4+C3H5-T     <=> B1E2M4J         9.45E+02    2.67   6850
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

B13DE2M+H       <=> B1E2M3J         4.000E+013 0.000  1300.0
!<C4H6+H<=>C4H71-3, SUBMECHANISM
C4H612+CH3      <=> B1E2M3J         1.76E+04  2.48   6130
!<EXTERNAL CH3 ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN.
38 (4) (2006) 250-275.

B13DE2M+H       <=> B1E3M3J         4.24E+11  0.51   1230
!<EXTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
(4) (2006) 250-275.
B12DE3M+H       <=> B1E3M3J         4.24E+11  0.51   1230
!<EXTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
(4) (2006) 250-275.

B13DE2M+H       <=> B1E3MJ          2.50E+11  0.51   2620
!<INTERNAL H ATOM ADDITION TO PROPENE, H.J. CURRAN, INT. J. CHEM. KIN. 38
(4) (2006) 250-275.
C2H3+C3H6       <=> B1E3MJ          9.45E+02    2.67   6850
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>
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!! R+HO2 = RO+OH
B1E2M3J+HO2     <=> B1E2M3OJ+OH     7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
B1E2M3J+CH3O2   <=> B1E2M3OJ+CH3O   7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
CH3CHO+C3H5-T   <=> B1E2M3OJ        9.45E+02   2.67   6850
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

B1E2M3J+HO2     <=> B2E2M1OJ+OH     7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
B1E2M3J+CH3O2   <=> B2E2M1OJ+CH3O   7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
CH2O+C4H72-2    <=> B2E2M1OJ        8.80E+03   2.48   6.1E+03
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

B1E3M3J+HO2     <=>  B1E3M3OJ+OH    7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
B1E3M3J+CH3O2   <=>  B1E3M3OJ+CH3O  7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
C2H3+CH3COCH3   <=>  B1E3M3OJ       9.45E+02   2.67   6850
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

B1E3M3J+HO2     <=>  B2E3M1OJ+OH    7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
B1E3M3J+CH3O2   <=>  B2E3M1OJ+CH3O  7.000E+012     0.000   -1000.0
!<C3H5-A+HO2, SUBMECHANISM
CH2O+IC4H7-I1    <=>  B2E3M1OJ       8.80E+03   2.48   6.1E+03
!<INTERNAL ADDITION TWO LARGE SPECIES J. P. ORME, H. J. CURRAN,* AND J.
M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131>

!REF: ANALOGY C2H3+O2 KLIPPENSTEIN
IC4H7-I1+O2<=>CH3COCH3+HCO                          3.100E+031    -5.944
5748.4
IC4H7-I1+O2<=>TC3H6CHO+O                            5.380E+018    -2.140
5142.9
IC4H7-I1+O2<=>IC3H5CHO+OH                           2.700E+019    -2.140
5142.9

!REF: THE SAME AS ALLYL+HO2
H15DE25DM-A+HO2<=>H15DE25DM-AO+OH                       1.000E+011
0.000       0.0
PLOG/      0.0100     9.04E+12    -0.14321    -1454.5492/
PLOG/      0.1000     2.20E+13    -0.26143    -1327.89059/
PLOG/      1.0000     1.28E+13    -0.1856        -1270.28914/
PLOG/     10.0000     7.09E+06    1.66007     -4481.39345/
PLOG/    100.0000     1.07E+05    2.24459     -5314.99428/
!
!!Estimate based on Curran IJCK 2006, 38, 250.
H15DE2M-T+CH2O<=>H15DE25DM-AO                         2.5E+010      0.00
4786.58
```

```
H15DE25DM-S+HO2<=>H15DE25DM-SO+OH                          1.000E+011
0.000       0.0
PLOG/      0.0100     9.04E+12    -0.14321    -1454.5492/
PLOG/      0.1000     2.20E+13    -0.26143    -1327.89059/
PLOG/      1.0000     1.28E+13    -0.1856        -1270.28914/
PLOG/     10.0000     7.09E+06    1.66007     -4481.39345/
PLOG/    100.0000     1.07E+05    2.24459     -5314.99428/
!
!Estimate based on Curran IJCK 2006, 38, 250.
IC3H5CHO+IC4H7<=>H15DE25DM-SO                               2.5E+010
0.00    6329.74
C3H5-T+IC4H7CHO<=>H15DE25DM-SO                              2.5E+010
0.00    15526.42
!
!  remove the following reaction
!  another reaction of ic4h7cho + oh is already present in the bc5h10
mechanism below
!IC4H7CHO+OH=>CH2CHO+C3H4-A+H2O                             5.064E+07
2.46     729.44
!
!REF:
!IC4H8<=>C3H5-T+CH3                                  1.920E+066   -14.220
128100.0
!IC4H8<=>IC4H7+H                                    3.070E+055   -11.490
114300.0
!IC4H8+H<=>C3H6+CH3                                 5.680E+033    -5.720
20000.0

!REF:ANALOGY WITH TSANG '92: C3H6+R<=>PRODUCTS
!IC4H8+H<=>IC4H7+H2                                 3.400E+005     2.500
2492.0

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS
!IC4H8+O=>CH2CO+CH3+CH3                             3.330E+007     1.760
76.0

!REF:
!IC4H8+O=>IC3H6CO+H+H                               1.660E+007     1.760
76.0

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS
!IC4H8+O<=>IC4H7+OH                                 1.206E+011     0.700
7633.0

!REF:
!IC4H8+CH3<=>IC4H7+CH4                              4.420E+000     3.500
5675.0
!IC4H8+HO2<=>IC4H7+H2O2                             1.928E+004     2.600
13910.0

!REF:ANALOGY WITH RH+RO2 --> R+RO2H
IC4H8+O2CHO<=>IC4H7+HO2CHO                         1.928E+004     2.600
13910.0
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!REF:
!IC4H8+O2<=>IC4H7+HO2                                  6.000E+012     0.000
39900.0

!REF:WESTBROOK AND PITZ ESTIMATE 1983
IC4H8+C3H5-A<=>IC4H7+C3H6                             7.940E+011     0.000
20500.0
IC4H8+C3H5-S<=>IC4H7+C3H6                             7.940E+011     0.000
20500.0
IC4H8+C3H5-T<=>IC4H7+C3H6                             7.940E+011     0.000
20500.0
!IC4H8+OH<=>IC4H7+H2O                                  5.200E+006     2.000
-298.0
!IC4H8+O<=>IC3H7+HCO                                   1.580E+007     1.760
-1216.0

!REF:
IC4H8+CH3O2<=>IC4H7+CH3O2H                            1.928E+004     2.600
13910.0

!!REF:BALDWIN, R. R., DEAN, C. E., AND WALKER, R. W., JCS FARADAY 2, 82,
1445 (1986)
!IC4H8+HO2<=>IC4H8O+OH                                 1.290E+012     0.000
13340.0

!!REF:ANOLOGY WITH BOZZELLI C3H5-A+O2 @ 10 ATM
!IC4H7+O2<=>IC3H5CHO+OH                                2.470E+013    -0.450
23020.0
!IC4H7+O2<=>CH3COCH2+CH2O                              7.140E+015    -1.210
21050.0
!IC4H7+O2=>C3H4-A+CH2O+OH                              2.180E+021    -2.850
30755.0

!REF:
IC4H7+O<=>IC3H5CHO+H                                  6.030E+013     0.000
0.0
!IC4H7<=>C3H4-A+CH3                                    1.230E+047    -9.740
74260.0
!CH3O2+IC4H7<=>CH3O+IC4H7O                             7.000E+012     0.000
-1000.0
!IC4H7+HO2<=>IC4H7O+OH                                 7.000E+012     0.000
-1000.0
!C3H5-T+CH2O<=>IC4H7O                                  1.000E+011     0.000
12600.0

!REF:EA<=>8.6+7 (RING STRAIN+EABS OF PRIMARY H BY RO)
IC4H7O<=>IC4H6OH                                      1.391E+011     0.000
15600.0
!IC4H7O<=>IC3H5CHO+H                                   5.000E+013     0.000
29100.0

!REF:ANALOGY C3H5-A+X --> PRODUCTS
IC4H6OH+H2<=>IC4H7OH+H                                2.160E+004     2.380
18990.0
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!REF:
IC4H7OH+O2<=>IC4H6OH+HO2                          6.000E+013     0.000
39900.0

!REF:RATE CONSTANT ANALOGY TO C3H5-A+CH2O (X 5)
IC4H6OH+CH2O<=>IC4H7OH+HCO                        6.300E+008     1.900
18190.0

!REF:CURRAN ESTIMATE
IC4H6OH+IC4H8<=>IC4H7OH+IC4H7                     4.700E+002     3.300
19840.0
IC4H6OH+H<=>IC4H7OH                               1.000E+014     0.000
0.0
IC4H6OH+H2O2<=>IC4H7OH+HO2                        7.830E+005     2.050
13580.0
C3H4-A+CH2OH<=>IC4H6OH                            1.000E+011     0.000
9200.0

!REF:FROM BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21, 411--429, 1992
IC4H7O+O2<=>IC3H5CHO+HO2                          3.000E+010     0.000
1649.0

!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986

!REF:ANALOGY CH3O+X --> CH2O+HX
IC4H7O+HO2<=>IC3H5CHO+H2O2                        3.000E+011     0.000
0.0
IC4H7O+CH3<=>IC3H5CHO+CH4                         2.400E+013     0.000
0.0
IC4H7O+O<=>IC3H5CHO+OH                            6.000E+012     0.000
0.0
IC4H7O+OH<=>IC3H5CHO+H2O                          1.810E+013     0.000
0.0
IC4H7O+H<=>IC3H5CHO+H2                            1.990E+013     0.000
0.0

!!REF:CURRAN ESTIMATE
!IC3H5CHO+OH<=>IC3H5CO+H2O                         2.690E+010     0.760
-340.0

!REF:FROM J. MENDES CALCULATED FOR ALDEHYDES
IC3H5CHO+OH<=>IC3H5CO+H2O                         61329.94775     2.65419
-4586.39996

!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X
!IC3H5CHO+HO2<=>IC3H5CO+H2O2                       1.000E+012     0.000
11920.0
!IC3H5CHO+CH3<=>IC3H5CO+CH4                        3.980E+012     0.000
8700.0
IC3H5CHO+O<=>IC3H5CO+OH                           7.180E+012     0.000
1389.0

!REF:FROM J. MENDES CALCULATED FOR ALDEHYDES
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IC3H5CHO+HO2<=>IC3H5CO+H2O2                          1.1773E-4      4.91966
3684.27444
IC3H5CHO+CH3<=>IC3H5CO+CH4                           1.24879        3.63386
4328.93484

!REF:
IC3H5CHO+O2<=>IC3H5CO+HO2                            2.000E+013     0.000
40700.0

!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X
!IC3H5CHO+H<=>IC3H5CO+H2                             2.600E+012     0.000
2600.0
IC3H5CO<=>C3H5-T+CO                                  1.278E+020    -1.890
34460.0

!REF: FROM J. MENDES CALCULATION FOR ALDEHYDES
IC3H5CHO+H<=>IC3H5CO+H2                              714740.3558    2.35674
1577.16272

!REF:ANALOGY WITH C3H5-A+CH3 --> 1-C4H8 TSANG 91 (PROPENE).
TC3H6OCHO+OH<=>TC3H6CHO+HO2                          2.018E+017    -1.200
21010.0

!REF:CURRAN AND GAFFURI, 1995.
TC3H6OCHO<=>CH3COCH3+HCO                             3.980E+013     0.000
9700.0

!REF:
IC3H5CHO+H<=>TC3H6CHO                                1.300E+013     0.000
1200.0
IC3H6CO+H<=>TC3H6CHO                                 1.300E+013     0.000
4800.0

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES
TC3H6CHO+H2<=>IC3H7CHO+H                             2.160E+005     2.380
18990.0
!IC4H7O+OH<=>IC4H7OOH                                1.000E+011     0.000
0.0
IC4H7O+H<=>IC4H7OH                                   4.000E+013     0.000
0.0

!REF:ANALOGY WITH IC4H9 --> IC4H8+H
IC4H7OH+H<=>IC4H8OH                                  1.000E+013     0.000
1200.0

!REF:ANALOGY WITH HCO+H2 --> CH2O+H

!REF:(TSANG/ HAMPSON 86) X 5
IC4H7O+H2<=>IC4H7OH+H                                9.050E+006     2.000
17830.0

!REF:CURRAN ESTIMATE
IC4H7+OH<=>IC4H7OH                                   3.000E+013     0.000
0.0
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IC4H7OH+HCO<=>IC4H7O+CH2O                          3.020E+011     0.000
18160.0

!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES
TC3H6CHO+CH2O<=>IC3H7CHO+HCO                       2.520E+008     1.900
18190.0
TC3H6CHO+IC4H8<=>IC3H7CHO+IC4H7                    4.700E+002     3.300
19840.0

!REF:ANALOGY TO 1C4H8+OH
IC3H6CO+OH<=>IC3H7+CO2                             1.730E+012     0.000
-1010.0

!REF:CURRAN ESTIMATE
TC3H6CHO+OH<=>TC3H6OHCHO                           5.000E+013     0.000
0.0

!REF:!TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
C3H6OH2-1+HCO<=>TC3H6OHCHO                         1.810E+013     0.000
0.0

!REF:ANALOGY WITH CH3CHOH --> CH3CHO+H.
 !REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13
CH3COCH3+H<=>C3H6OH2-1                             8.000E+012     0.000
9500.0
C2H5CHO+H<=>C3H6OH1-2                              8.000E+012     0.000
9500.0

!REF:BASED ON IC4H8+H<=>IC4H9
IC3H5OH+H<=>C3H6OH2-1                              6.250E+011     0.510
4020.0

!REF:REVERSE BY ANALOGY HCO+OH --> PRODUCTS
C3H5-T+OH<=>IC3H5OH                                5.000E+013     0.000
0.0

!REF:
TC3H6CHO+O2<=>TC3H6O2CHO                           1.990E+017    -2.100
0.0
TC3H6O2CHO<=>IC3H5O2HCHO                           6.000E+011     0.000
29880.0
TC3H6O2CHO<=>TC3H6O2HCO                            1.000E+011     0.000
25750.0

!REF:REVERSE ANALOGY IC4H8+CH3 --> NEOC5H11.

!REF:SLAGLE ET AL. J. PHYS. CHEM. 1991, 95
IC3H5CHO+HO2<=>IC3H5O2HCHO                         2.230E+011     0.000
10600.0

!REF:
TC3H6O2HCO=>CH3COCH3+CO+OH                         4.244E+018    -1.430
4800.0
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!REF:!MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS. CHEM. 1990, 94, 3016
C3H6OH2-1+O2<=>CH3COCH3+HO2                          1.500E+012     0.000
5000.0
C3H6OH1-2+O2<=>C2H5CHO+HO2                           1.500E+012     0.000
5000.0

!REF:CURRAN ESTIMATE
IC3H6CO+OH<=>C3H6OH2-1+CO                            2.000E+012     0.000
-1010.0

!REF:!LOHDI, Z.H.; WALKER, R.W.; J. CHEM. SOC. FARAD. 1991 87, 2361
(C3H5-A+HO2) (X 0.5)
TC3H6CHO+HO2<=>IC3H7CHO+O2                           3.675E+012     0.000
1310.0

!REF:CURRAN ESTIMATE
TC3H6CHO+CH3<=>IC3H5CHO+CH4                          3.010E+012    -0.320
-131.0

!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95
TC4H8CHO<=>IC3H5CHO+CH3                              1.000E+013     0.000
26290.0
TC4H8CHO<=>IC4H8+HCO                                 8.520E+012     0.000
20090.0

!REF:CURRAN ESTIMATE
TC4H8CHO+O2<=>O2C4H8CHO                              2.000E+012     0.000
0.0
O2C4H8CHO<=>O2HC4H8CO                                2.160E+011     0.000
15360.0
IC4H8O2H-T+CO<=>O2HC4H8CO                            1.500E+011     0.000
4809.0

!REF:PITZ ESTIMATE
IC4H7O+IC4H8<=>IC4H7OH+IC4H7                         2.700E+011     0.000
4000.0

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

!REF:CURRAN ESTIMATE
IC4H8+CH2CCH2OH<=>IC4H7+C3H5OH                       7.940E+011     0.000
20500.0
CH2CCH2OH+H2O2<=>C3H5OH+HO2                          3.010E+009     0.000
2583.0
C3H5OH+OH<=>CH2CCH2OH+H2O                            5.060E+012     0.000
5960.0
C3H5OH+H<=>CH2CCH2OH+H2                              3.900E+005     2.500
5821.0
C3H5OH+O2<=>CH2CCH2OH+HO2                            4.000E+013     0.000
60690.0
C3H5OH+CH3<=>CH2CCH2OH+CH4                           2.400E+011     0.000
8030.0
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!REF:CURRAN ESTIMATE
CH2CCH2OH+CH3<=>IC4H7OH                           3.000E+013     0.000
0.0
CH2CCH2OH+H<=>C3H5OH                              1.000E+014     0.000
0.0
CH2CCH2OH+O2=>CH2OH+CO+CH2O                       4.335E+012     0.000
0.0
CH2CCH2OH<=>C2H2+CH2OH                            2.163E+040    -8.310
45110.0
C3H5-A+C2H2<=>C*CC*CCJ                            1.000E+012     0.000
6883.4
C3H5-A+C2H3=>C5H6+H+H                             1.600E+035   -14.000
61137.7
C3H4-A+C3H3<=>C6H6+H                              1.400E+012     0.000
9990.4

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H6+C2H3=>C6H6+H2+H                              5.620E+011     0.000
3240.0
C4H5-N+C2H2<=>C6H6+H                              1.600E+016    -1.330
5400.0
C4H5-N+C2H3<=>C6H6+H2                             1.840E-013     7.070
-3611.0
C4H5-2+C2H2<=>C6H6+H                              5.000E+014     0.000
25000.0
C4H5-2+C2H4<=>C5H6+CH3                            5.000E+014     0.000
25000.0
C6H2+H<=>C6H3                                     1.100E+030    -4.920
10800.0
C6H3+H<=>C4H2+C2H2                                2.800E+023    -2.550
10780.0
C6H3+H<=>L-C6H4                                   3.400E+043    -9.010
12120.0
C6H3+H<=>C6H2+H2                                  3.000E+013     0.000
0.0
C6H3+OH<=>C6H2+H2O                                4.000E+012     0.000
0.0
L-C6H4+H<=>C6H5                                   1.700E+078   -19.720
31400.0
L-C6H4+H<=>C-C6H4+H                               1.400E+054   -11.700
34500.0
L-C6H4+H<=>C6H3+H2                                1.330E+006     2.530
9240.0
L-C6H4+OH<=>C6H3+H2O                              3.100E+006     2.000
430.0
C-C6H4+H<=>C6H5                                   2.400E+060   -13.660
29500.0
C4H3-N+C2H2<=>L-C6H4+H                            2.500E+014    -0.560
10600.0
C4H3-N+C2H2<=>C6H5                                9.600E+070   -17.770
31300.0
C4H3-N+C2H2<=>C-C6H4+H                            6.900E+046   -10.010
30100.0
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!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)
C4H3-I+CH3<=>C5H6                                   1.000E+012     0.000
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H2+C2H<=>C6H2+H                                   9.600E+013     0.000
0.0
C4H2+C2H<=>C6H3                                     4.500E+037    -7.680
7100.0
C4H4+C2H<=>L-C6H4+H                                 1.200E+013     0.000
0.0

!REF:WANG ET AL. C&F, 110: 173. 1994
C6H5+H(+M)<=>C6H6(+M)                               1.000E+014     0.000
0.0
LOW/                                                6.600E+075   -16.300
7000.0/
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                                  6.300E+013     0.000
60000.0

!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)
C6H6+O<=>C6H5O+H                                    2.200E+013     0.000
4530.0

!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)
C6H6+O<=>C6H5+OH                                    2.000E+013     0.000
14700.0

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
C6H6+H<=>C6H5+H2                                    2.500E+014     0.000
16000.0

!REF:ESTIMATED
C6H6+CH3<=>C6H5+CH4                                 7.320E+012     0.000
18920.0

!REF:ESTIMATED
C6H6+HO2<=>C6H5+H2O2                                5.500E+012     0.000
28900.0

!REF:CHEN&BOZ J. PHYS. CHEM. A 108: 4632 - 4652 2004
C6H6+OH<=>C6H5+H2O                                  1.200E+000     4.100
-301.0

!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
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!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
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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
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!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
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!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
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!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                                      3.200E+013    -0.170
440.0
C5H5+O<=>C5H4O+H                                        5.800E+013    -0.020
20.0
C5H5+OH<=>C5H5OH                                        6.500E+014    -0.850
-2730.0
DUP
C5H5+OH<=>C5H5OH                                        1.100E+043    -8.760
18730.0
DUP
C5H5+OH<=>C5H5OH                                        1.100E+059   -13.080
33450.0
DUP
C5H5+OH<=>C5H4OH+H                                      3.500E+057   -12.180
48350.0

!REF:RISTORI ET AL. COMBUST. SCI. AND TECH 2001. VOL. 167. PP. 223-256
C5H5+OH<=>C4H6+CO                                       4.000E+014     0.000
4500.0
C5H5+HO2<=>C5H5O+OH                                     6.300E+029    -4.690
11650.0

!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                                     6.000E+018    -2.480
10970.0

!REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000
C4H4O+H<=>C3H5-A+CO                                     6.600E+013    -0.020
2740.0
DUP
C4H4O+H<=>C3H5-A+CO                                     5.900E+006     2.000
1300.0
DUP
C4H4O+O<=>CH2CHO+HCCO                                   3.000E+008     1.450
-860.0
C4H4O+OH<=>C3H5-A+CO2                                   3.000E+012     0.000
0.0

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

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

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

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

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

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

!REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-
418
CJ*CC*CC*O<=>C2H2+CJ*CC*O                         3.000E+013     0.000
43710.0
CJ*CC*O<=>C2H3CO                                  1.400E+009     0.980
32100.0
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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
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!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 & BOZZELI J PHYS CHEM A 102: 3537 1998
C5H6+H<=>C5H7                                       2.400E+073   -17.850
31500.0
C5H6+H<=>C*CCJC*C                                   1.100E+014    -0.160
3100.0
C5H6+O<=>C5H5O+H                                    8.900E+012    -0.150
590.0
DUP
C5H6+O<=>C5H5O+H                                    5.600E+012    -0.060
200.0
DUP
C5H6+OH<=>C*CCJC*COH                                1.100E+013    -0.070
870.0
C5H6+HO2<=>C5H7+O2                                  1.300E+015    -1.070
9530.0
C5H6+HCO<=>C5H5+CH2O                                1.080E+008     1.900
16000.0
C5H6+C2H3<=>C6H6+CH3                                2.100E+067   -16.080
42460.0

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

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

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

!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
C*CC*CC+H<=>C*CC*CCJ+H2                             7.000E+006     2.000
5000.0
C*CC*CC+OH<=>C*CC*CCJ+H2O                           7.000E+006     2.000
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C*CCJC*C+O2<=>C2H3CHO+CH2CHO                        1.200E+036    -7.250
33600.0
C*CC*CCJ+H<=>C4H5-N+CH3                             2.900E+026    -2.180
36770.0
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!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
C*CCJC*C+O<=>C2H3CHO+C2H3                          2.000E+014     0.000
0.0

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

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C*CC*CCJ+OH<=>C*CC*CCOH                            1.500E+013     0.000
0.0
C*CC*CCJ+O2<=>C*CCJC*O+CH2O                        8.200E+010     0.180
9140.0
C*CC*CCOH+H<=>C4H6+CH2OH                           2.500E+034    -6.120
16250.0

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

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
OC5H7O+O2<=>OC4H6O+HOCO                            6.300E+005    -7.250
33600.0
C*CCJC*COH+O2<=>HOC*CC*O+CH2CHO                    1.200E+036    -7.250
33600.0
HOC*CC*O+OH<=>HOC*CCJ*O+H2O                        2.690E+010     0.760
-340.0
HOC*CC*O+HO2<=>HOC*CCJ*O+H2O2                      1.000E+012     0.000
11920.0
HOC*CC*O+CH3<=>HOC*CCJ*O+CH4                       3.980E+012     0.000
8700.0
HOC*CC*O+O<=>HOC*CCJ*O+OH                          7.180E+012     0.000
1389.0
HOC*CC*O+O2<=>HOC*CCJ*O+HO2                        2.000E+013     0.000
40700.0
HOC*CC*O+H<=>HOC*CCJ*O+H2                          2.600E+012     0.000
2600.0

!REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO
C2H2OH+CO<=>HOC*CCJ*O                              1.510E+011     0.000
4810.0

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

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

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
C*CCJC*O<=>C3H5-A+CO                               6.100E+005     0.920
-1120.0
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C*CCJC*O+O2<=>C2H3CHO+HOCO                              1.200E+036    -7.250
33600.0

!REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013
HOCO<=>CO+OH                                            6.300E+032    -5.960
32470.0
PLOG/      0.0010     1.550E-008     2.930      8768.0/
PLOG/      0.0030     1.770E+003     0.340     18076.0/
PLOG/      0.0296     2.020E+013    -1.870     22755.0/
PLOG/      0.0987     1.680E+018    -3.050     24323.0/
PLOG/      0.2961     2.500E+024    -4.630     27067.0/
PLOG/      0.9869     4.540E+026    -5.120     27572.0/
PLOG/      2.9607     7.120E+028    -5.600     28535.0/
PLOG/      9.8690     5.480E+029    -5.700     28899.0/
PLOG/     29.6070     9.890E+031    -6.190     30518.0/
PLOG/     98.6900     5.740E+033    -6.530     32068.0/
PLOG/    296.0700     2.610E+033    -6.290     32231.0/
PLOG/    986.9000     6.300E+032    -5.960     32470.0/
HOCO<=>CO2+H                                            1.897E+038    -8.047
34240.0
PLOG/      0.0010     4.758E+018    -3.817     17676.0/
PLOG/      0.0030     2.225E+020    -4.149     19037.0/
PLOG/      0.0099     7.564E+021    -4.434     20325.0/
PLOG/      0.0296     9.107E+024    -5.189     22419.0/
PLOG/      0.0987     3.144E+029    -6.376     25233.0/
PLOG/      0.2961     1.150E+032    -7.037     26662.0/
PLOG/      0.9869     1.069E+036    -8.107     29064.0/
PLOG/      2.9607     2.438E+036    -8.153     29336.0/
PLOG/      9.8690     6.663E+035    -7.919     29217.0/
PLOG/     29.6070     1.723E+038    -8.506     31273.0/
PLOG/     98.6900     3.007E+041    -9.290     33966.0/
PLOG/    296.0700     6.767E+036    -7.832     31613.0/
PLOG/    986.9000     1.897E+038    -8.047     34240.0/
C6H10+H<=>C6H9-A+H2                                     6.752E+005     2.360
207.0
C6H10+CH3<=>C6H9-A+CH4                                  7.380E+000     3.310
4002.0
C6H10+O<=>C6H9-A+OH                                     1.320E+006     2.430
1210.0
C6H10+OH<=>C6H9-A+H2O                                   5.528E+004     2.640
-1919.0
C4H6+C2H3<=>C6H9-A                                      8.800E+005     2.500
6130.0

!REF:  FRIDLYAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776
C6H10<=>C3H5-A+C3H5-A                                   4.900E+022    -2.060
63355.5
PLOG/      1.0000     5.070E+047    -9.700     72680.0/
PLOG/      4.0000     4.220E+039    -7.300     69390.0/
PLOG/     10.0000     2.120E+035    -6.000     67620.0/
C3H5-A+C3H5-A<=>C3H4-A+C3H6                             9.550E+040    -9.300
12470.0
PLOG/      1.0000     4.770E+040    -9.300     12470.0/
PLOG/      4.0000     3.970E+032    -6.800      9180.0/
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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

!Pressure dependent unimolecular decomposition rate constants calculated
by JB 6/10/2013 based on LJ parameters from A. W. Jasper, J. A. Miller.
Combust. Flame (2013)
NC5H12 <=> NC3H7+C2H5 5.203E+024 -2.071 88080.0
PLOG  / 1.000E-002 1.180E+096 -23.17 126046. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E-001 1.855E+089 -20.90 125630. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+000 3.550E+076 -17.02 120458. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 3.475E+071 -15.54 117854. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 2.160E+064 -13.43 113815. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+001 4.550E+058 -11.79 110456. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+001 1.020E+053 -10.15 106996. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 5.000E+001 9.000E+045  -8.13 102538. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12 <=> PC4H9+CH3 1.451E+022 -1.522 89100.0
PLOG  / 1.000E-002 7.090E+092 -22.46 126235. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E-001 4.830E+086 -20.36 126331. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+000 3.240E+074 -16.63 121640. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 4.030E+069 -15.18 119142. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 3.000E+062 -13.09 115199. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 6.470E+056 -11.44 111875. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+001 1.360E+051  -9.80 108418. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 5.000E+001 9.740E+043  -7.75 103923. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12 <=> C5H11-1+H 4.205E+017 -0.390 101180.0
PLOG  / 1.000E-002 1.990E+074 -17.75 124798. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E-001 5.720E+076 -18.01 131106. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E+000 4.420E+072 -16.46 132942. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
```

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PLOG  / 2.000E+000 4.560E+069 -15.52 132148. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 2.640E+064 -13.92 130026. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 3.800E+059 -12.48 127648. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 1.440E+054 -10.89 124707. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 3.280E+046  -8.67 120241. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12 <=> C5H11-2+H 2.493E+018 -0.632 97930.0
PLOG  / 1.000E-002 6.930E+079 -19.24 125716. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E-001 7.690E+079 -18.83 130425. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+000 2.340E+073 -16.63 130412. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 5.640E+069 -15.52 129087. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 6.770E+063 -13.74 126353. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 4.300E+058 -12.21 123622. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 1.060E+053 -10.57 120451. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 2.500E+045  -8.36 115883. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12 <=> C5H11-3+H 1.257E+018 -0.633 97930.0
PLOG  / 1.000E-002 3.490E+079 -19.24 125716. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E-001 3.880E+079 -18.84 130425. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+000 1.180E+073 -16.63 130412. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 2.840E+069 -15.52 129087. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 3.410E+063 -13.74 126353. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 2.170E+058 -12.21 123622. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 5.320E+052 -10.57 120451. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 1.260E+045  -8.36 115883. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12+H<=>C5H11-1+H2                             3.490E+005     2.690
6450.0
NC5H12+H<=>C5H11-2+H2                             2.600E+006     2.400
4471.0
NC5H12+H<=>C5H11-3+H2                             1.300E+006     2.400
4471.0
```

NC5H12+OH<=>C5H11-1+H2O 1.054E+010 0.970
1586.0
NC5H12+OH<=>C5H11-2+H2O 9.340E+007 1.610
-35.0
NC5H12+OH<=>C5H11-3+H2O 4.670E+007 1.610
-35.0
NC5H12+O<=>C5H11-1+OH 1.130E+014 0.000
7850.0
NC5H12+O<=>C5H11-2+OH 5.620E+013 0.000
5200.0
NC5H12+O<=>C5H11-3+OH 2.810E+013 0.000
5200.0
NC5H12+CH3<=>C5H11-1+CH4 9.040E-001 3.650
7154.0
NC5H12+CH3<=>C5H11-2+CH4 1.680E+005 2.133
7574.0
NC5H12+CH3<=>C5H11-3+CH4 8.400E+004 2.133
7574.0
NC5H12+HO2<=>C5H11-1+H2O2 4.080E+001 3.590
17160.0
NC5H12+HO2<=>C5H11-2+H2O2 1.264E+002 3.370
13720.0
NC5H12+HO2<=>C5H11-3+H2O2 6.320E+001 3.370
13720.0
NC5H12+CH3O2<=>C5H11-1+CH3O2H 1.386E+000 3.970
18280.0
NC5H12+CH3O2<=>C5H11-2+CH3O2H 2.037E+001 3.580
14810.0
NC5H12+CH3O2<=>C5H11-3+CH3O2H 1.019E+001 3.580
14810.0
NC5H12+C2H5<=>C5H11-1+C2H6 1.000E+011 0.000
13400.0
NC5H12+C2H5<=>C5H11-2+C2H6 1.000E+011 0.000
10400.0
NC5H12+C2H5<=>C5H11-3+C2H6 5.000E+010 0.000
10400.0
NC5H12+C2H3<=>C5H11-1+C2H4 1.000E+012 0.000
18000.0
NC5H12+C2H3<=>C5H11-2+C2H4 8.000E+011 0.000
16800.0
NC5H12+C2H3<=>C5H11-3+C2H4 4.000E+011 0.000
16800.0
NC5H12+C5H11-1<=>C5H11-2+NC5H12 1.000E+011 0.000
10400.0
NC5H12+C5H11-1<=>C5H11-3+NC5H12 5.000E+010 0.000
10400.0
NC5H12+C5H11-2<=>C5H11-3+NC5H12 5.000E+010 0.000
12300.0
NC5H12+O2CHO<=>C5H11-1+HO2CHO 1.386E+000 3.970
18280.0
NC5H12+O2CHO<=>C5H11-2+HO2CHO 2.037E+001 3.580
14810.0
NC5H12+O2CHO<=>C5H11-3+HO2CHO 1.019E+001 3.580
14810.0

```
NC5H12+CH3O<=>C5H11-1+CH3OH                          3.000E+011     0.000
7000.0
NC5H12+CH3O<=>C5H11-2+CH3OH                          2.200E+011     0.000
5000.0
NC5H12+CH3O<=>C5H11-3+CH3OH                          1.100E+011     0.000
5000.0
NC5H12+O2<=>C5H11-1+HO2                              4.200E+013     0.000
52800.0
NC5H12+O2<=>C5H11-2+HO2                              2.800E+013     0.000
50160.0
NC5H12+O2<=>C5H11-3+HO2                              1.400E+013     0.000
50160.0

!A. Comandini, I. A. Awan, J. A. Manion. Chem. Phys. Lett. 2012, 552, 20-
26
C5H11-1<=>C2H4+NC3H7                                 3.236E+12     0.323
28808.4
PLOG/    0.1        4.410E+03      2.192    18827.0 /
PLOG/    1.0        8.060E+20     -2.628    29232.0 /
PLOG/   10.0        2.170E+28     -4.578    34864.0 /
PLOG/  100.0        6.470E+24     -3.383    34388.0 /
PLOG/ 1000.0        2.340E+17     -1.123    31176.0 /

C5H11-1<=>H+C5H10-1                                  2.042E+10     0.950
33810.2
PLOG/    0.1        3.240E-14      7.022    15354.0 /
PLOG/    1.0        5.100E+12     -0.402    29991.0 /
PLOG/   10.0        4.070E+27     -4.483    39814.0 /
PLOG/  100.0        1.020E+26     -3.794    40806.0 /
PLOG/ 1000.0        6.520E+16     -0.987    36957.0 /

C5H11-1<=>C5H11-2                                    1.148E+01     3.033
15313.4
PLOG/    0.1        1.610E+10     -0.128    16305.0 /
PLOG/    1.0        2.880E+17     -2.073    21414.0 /
PLOG/   10.0        5.090E+18     -2.284    23337.0 /
PLOG/  100.0        1.380E+14     -0.838    21871.0 /
PLOG/ 1000.0        1.600E+08      0.954    19221.0 /

C5H11-1<=>C5H11-3                                    3.890E-12     6.843
18781.0
PLOG/    0.1        6.080E-15      6.876    11901.0 /
PLOG/    1.0        7.680E+07      0.667    25012.0 /
PLOG/   10.0        1.260E+19     -2.350    32938.0 /
PLOG/  100.0        1.160E+16     -1.256    33072.0 /
PLOG/ 1000.0        6.060E+06      1.570    29120.0 /

C5H11-2<=>C5H11-3                                    2.754E+10     0.712
41872.3
PLOG/    0.1        4.800E-04      3.725    28298.0 /
PLOG/    1.0        3.410E+22     -3.517    42976.0 /
PLOG/   10.0        1.570E+32     -6.005    50425.0 /
PLOG/  100.0        3.120E+24     -3.514    48305.0 /
PLOG/ 1000.0        1.590E+14     -0.404    43709.0 /
```

```
C5H11-2<=>C3H6+C2H5                                     4.074E+12     0.272
29140.3
PLOG/    0.1        8.540E+25     -4.241    31303.0 /
PLOG/    1.0        2.340E+31     -5.581    35992.0 /
PLOG/   10.0        4.630E+28     -4.592    36186.0 /
PLOG/  100.0        3.770E+20     -2.108    32927.0 /
PLOG/ 1000.0        3.560E+14     -0.301    30124.0 /

C5H11-2<=>C5H10-1+H                                     2.239E+08     1.517
34750.2
PLOG/    0.1        8.260E+10     -0.118    29715.0 /
PLOG/    1.0        6.920E+26     -4.456    39997.0 /
PLOG/   10.0        3.810E+29     -4.969    43662.0 /
PLOG/  100.0        4.220E+20     -2.160    40523.0 /
PLOG/ 1000.0        5.050E+11      0.526    36461.0 /

C5H11-2<=>C5H10-2+H                                     2.710E+09     1.193
34513.5
PLOG/    0.1        2.797E+13     -0.833    30422.7 /
PLOG/    1.0        9.922E+27     -4.775    39987.0 /
PLOG/   10.0        8.504E+29     -5.063    43150.6 /
PLOG/  100.0        1.026E+21     -2.275    39953.2 /
PLOG/ 1000.0        3.141E+12      0.287    36068.2 /

C5H11-3<=>C4H8-1+CH3                                    2.951E+10     0.928
30048.5
PLOG/    0.1        1.310E+16     -1.137    29671.0 /
PLOG/    1.0        1.850E+25     -3.643    35787.0 /
PLOG/   10.0        1.010E+24     -3.130    36363.0 /
PLOG/  100.0        1.980E+16     -0.793    33017.0 /
PLOG/ 1000.0        2.100E+11      0.685    30583.0 /

C5H11-3<=>C5H10-2+H                                     1.274E+09     1.330
34417.9
PLOG/    0.1        5.119E+06      1.511    29138.7 /
PLOG/    1.0        4.068E+22     -2.949    38765.5 /
PLOG/   10.0        2.298E+25     -3.569    41777.2 /
PLOG/  100.0        8.104E+16     -0.983    38322.3 /
PLOG/ 1000.0        1.214E+10      1.047    35008.7 /

C5H10-1<=>C2H5+C3H5-A                                   9.864E+021    -2.086
75060.0
C5H10-1+H<=>C5H91-3+H2                                  3.376E+005     2.360
207.0
C5H10-1+H<=>C5H91-4+H2                                  1.300E+006     2.400
4471.0
C5H10-1+H<=>C5H91-5+H2                                  6.650E+005     2.540
6756.0
C5H10-1+O<=>C5H91-3+OH                                  6.600E+005     2.430
1210.0
C5H10-1+O<=>C5H91-4+OH                                  5.510E+005     2.450
2830.0
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C5H10-1+O<=>C5H91-5+OH 9.800E+005 2.430
4750.0
C5H10-1+OH<=>C5H91-3+H2O 2.764E+004 2.640
-1919.0
C5H10-1+OH<=>C5H91-4+H2O 4.670E+007 1.610
-35.0
C5H10-1+OH<=>C5H91-5+H2O 5.270E+009 0.970
1586.0
C5H10-1+CH3<=>C5H91-3+CH4 3.690E+000 3.310
4002.0
C5H10-1+CH3<=>C5H91-4+CH4 1.510E+000 3.460
5481.0
C5H10-1+CH3<=>C5H91-5+CH4 4.521E-001 3.650
7154.0
C5H10-1+O2<=>C5H91-3+HO2 2.200E+012 0.000
37220.0
C5H10-1+O2<=>C5H91-4+HO2 2.000E+013 0.000
49640.0
C5H10-1+O2<=>C5H91-5+HO2 3.000E+013 0.000
52290.0
C5H10-1+HO2<=>C5H91-3+H2O2 4.820E+003 2.550
10530.0
C5H10-1+HO2<=>C5H91-4+H2O2 9.640E+003 2.600
13910.0
C5H10-1+HO2<=>C5H91-5+H2O2 2.380E+004 2.550
16490.0
C5H10-1+CH3O2<=>C5H91-3+CH3O2H 4.820E+003 2.550
10530.0
C5H10-1+CH3O2<=>C5H91-4+CH3O2H 9.640E+003 2.600
13910.0
C5H10-1+CH3O2<=>C5H91-5+CH3O2H 2.380E+004 2.550
16490.0
C5H10-1+CH3O<=>C5H91-3+CH3OH 4.000E+001 2.900
8609.0
C5H10-1+CH3O<=>C5H91-4+CH3OH 1.450E+011 0.000
4571.0
C5H10-1+CH3O<=>C5H91-5+CH3OH 2.170E+011 0.000
6458.0
C5H10-2+H<=>C5H91-3+H2 1.730E+005 2.500
2492.0
C5H10-2+H<=>C5H92-4+H2 3.376E+005 2.360
207.0
C5H10-2+H<=>C5H92-5+H2 6.651E+005 2.540
6756.0
C5H10-2+O<=>C5H91-3+OH 4.410E+005 2.420
3150.0
C5H10-2+O<=>C5H92-4+OH 9.900E+005 2.430
1210.0
C5H10-2+O<=>C5H92-5+OH 9.800E+005 2.430
4750.0
C5H10-2+OH<=>C5H91-3+H2O 3.120E+006 2.000
-298.0
C5H10-2+OH<=>C5H92-4+H2O 2.764E+004 2.640
-1919.0

C5H10-2+OH<=>C5H92-5+H2O 5.270E+009 0.970
1586.0
C5H10-2+CH3<=>C5H91-3+CH4 2.210E+000 3.500
5675.0
C5H10-2+CH3<=>C5H92-4+CH4 3.690E+000 3.310
4002.0
C5H10-2+CH3<=>C5H92-5+CH4 4.521E-001 3.650
7154.0
C5H10-2+O2<=>C5H91-3+HO2 3.300E+012 0.000
39900.0
C5H10-2+O2<=>C5H92-4+HO2 2.200E+012 0.000
37220.0
C5H10-2+O2<=>C5H92-5+HO2 3.000E+013 0.000
52290.0
C5H10-2+HO2<=>C5H91-3+H2O2 9.639E+003 2.600
13910.0
C5H10-2+HO2<=>C5H92-4+H2O2 4.820E+003 2.550
10530.0
C5H10-2+HO2<=>C5H92-5+H2O2 2.380E+004 2.550
16490.0
C5H10-2+CH3O2<=>C5H91-3+CH3O2H 9.639E+003 2.600
13910.0
C5H10-2+CH3O2<=>C5H92-4+CH3O2H 4.820E+003 2.550
10530.0
C5H10-2+CH3O2<=>C5H92-5+CH3O2H 2.380E+004 2.550
16490.0
C5H10-2+CH3O<=>C5H91-3+CH3OH 9.000E+001 2.950
11990.0
C5H10-2+CH3O<=>C5H92-4+CH3OH 4.000E+001 2.900
8609.0
C5H10-2+CH3O<=>C5H92-5+CH3OH 2.170E+011 0.000
6458.0
C5H9O1-3+OH<=>C5H91-3+HO2 6.088E+015 -1.070
15720.0
C5H9O1-3+CH3O<=>C5H91-3+CH3O2 5.946E+017 -1.650
20480.0
C5H9O1-3+C2H5O<=>C5H91-3+C2H5O2 3.893E+014 -0.720
18330.0
C5H9O2-4+OH<=>C5H92-4+HO2 7.027E+015 -1.240
15890.0
C5H9O2-4+CH3O<=>C5H92-4+CH3O2 6.863E+017 -1.820
20650.0
C5H9O2-4+C2H5O<=>C5H92-4+C2H5O2 4.493E+014 -0.890
18490.0
C4H6+CH3<=>C5H91-3 1.000E+011 0.000
7800.0
C5H81-3+H<=>C5H91-3 2.500E+011 0.510
2620.0
C3H6+C2H3<=>C5H91-4 1.000E+011 0.000
7800.0
C2H4+C3H5-A<=>C5H91-5 1.000E+011 0.000
7800.0
C5H81-3+H<=>C5H92-4 4.240E+011 0.510
1230.0

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C2H4+C3H5-S<=>C5H92-5                                2.000E+011     0.000
7800.0
C5H9O1-3<=>C2H3CHO+C2H5                              3.131E+019    -1.850
10670.0
C5H9O1-3<=>C2H5CHO+C2H3                              1.417E+018    -1.560
23340.0
C5H81-3+OH<=>CH2O+C4H71-3                            1.000E+012     0.000
0.0
C5H81-3+OH<=>C2H3CHO+C2H5                            1.000E+012     0.000
0.0
C5H81-3+OH<=>CH3CHO+C3H5-S                           1.000E+012     0.000
0.0
C5H9O2-4<=>SC3H5CHO+CH3                              5.983E+015    -1.130
9941.0
C5H9O2-4<=>CH3CHO+C3H5-S                             1.073E+022    -2.660
29650.0
C5H10-2(+M)<=>CH3+C4H71-3(+M)                        6.486E+019    -1.367
76320.0
LOW/                                                 1.527E+104   -24.826
94800.0/
TROE/  5.301E-003  1.437E+002  1.677E+013  3.671E+003/
C5H11-1+O2<=>C5H10-1+HO2                             8.370E-001     3.590
11960.0
C5H11-2+O2<=>C5H10-1+HO2                             5.350E-001     3.710
9322.0
C5H11-2+O2<=>C5H10-2+HO2                             1.070E+000     3.710
9322.0
C5H11-3+O2<=>C5H10-2+HO2                             2.140E+000     3.710
9322.0
C5H11-1+HO2<=>C5H11O-1+OH                            9.000E+012     0.000
-1000.0
C5H11-2+HO2<=>C5H11O-2+OH                            9.000E+012     0.000
-1000.0
C5H11-3+HO2<=>C5H11O-3+OH                            9.000E+012     0.000
-1000.0
C5H11-1+CH3O2<=>C5H11O-1+CH3O                        9.000E+012     0.000
-1000.0
C5H11-2+CH3O2<=>C5H11O-2+CH3O                        9.000E+012     0.000
-1000.0
C5H11-3+CH3O2<=>C5H11O-3+CH3O                        9.000E+012     0.000
-1000.0
C5H11O2-1+NC5H12<=>C5H11O2H-1+C5H11-1                1.210E+013     0.000
20430.0
C5H11O2-2+NC5H12<=>C5H11O2H-2+C5H11-1                1.210E+013     0.000
20430.0
C5H11O2-3+NC5H12<=>C5H11O2H-3+C5H11-1                1.210E+013     0.000
20430.0
C5H11O2-1+NC5H12<=>C5H11O2H-1+C5H11-2                8.064E+012     0.000
17700.0
C5H11O2-2+NC5H12<=>C5H11O2H-2+C5H11-2                8.064E+012     0.000
17700.0
C5H11O2-3+NC5H12<=>C5H11O2H-3+C5H11-2                8.064E+012     0.000
17700.0
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C5H11O2-1+NC5H12<=>C5H11O2H-1+C5H11-3              4.032E+012     0.000
17700.0
C5H11O2-2+NC5H12<=>C5H11O2H-2+C5H11-3              4.032E+012     0.000
17700.0
C5H11O2-3+NC5H12<=>C5H11O2H-3+C5H11-3              4.032E+012     0.000
17700.0
C5H11-1+C5H11O2-1<=>C5H11O-1+C5H11O-1              9.000E+012     0.000
-1000.0
C5H11-1+C5H11O2-2<=>C5H11O-1+C5H11O-2              9.000E+012     0.000
-1000.0
C5H11-1+C5H11O2-3<=>C5H11O-1+C5H11O-3              9.000E+012     0.000
-1000.0
C5H11-2+C5H11O2-1<=>C5H11O-2+C5H11O-1              9.000E+012     0.000
-1000.0
C5H11-2+C5H11O2-2<=>C5H11O-2+C5H11O-2              9.000E+012     0.000
-1000.0
C5H11-2+C5H11O2-3<=>C5H11O-2+C5H11O-3              9.000E+012     0.000
-1000.0
C5H11-3+C5H11O2-1<=>C5H11O-3+C5H11O-1              9.000E+012     0.000
-1000.0
C5H11-3+C5H11O2-2<=>C5H11O-3+C5H11O-2              9.000E+012     0.000
-1000.0
C5H11-3+C5H11O2-3<=>C5H11O-3+C5H11O-3              9.000E+012     0.000
-1000.0
C5H11O2-1+C5H11O2-2=>O2+C5H11O-1+C5H11O-2         1.400E+016    -1.610
1860.0
C5H11O2-1+C5H11O2-3=>O2+C5H11O-1+C5H11O-3         1.400E+016    -1.610
1860.0
C5H11O2-1+CH3O2=>O2+C5H11O-1+CH3O                 1.400E+016    -1.610
1860.0
C5H11O2-1+C5H11O2-1=>O2+C5H11O-1+C5H11O-1         1.400E+016    -1.610
1860.0
C5H11O2H-1+HO2<=>C5H11O2-1+H2O2                    2.400E+012     0.000
10000.0
C5H11O2H-1+O2<=>C5H11O2-1+HO2                      3.746E+013    -0.791
33620.0
C5H11O2-2+CH3O2=>O2+C5H11O-2+CH3O                 1.400E+016    -1.610
1860.0
C5H11O2-2+C5H11O2-3=>C5H11O-2+C5H11O-3+O2         1.400E+016    -1.610
1860.0
C5H11O2-2+C5H11O2-2=>O2+C5H11O-2+C5H11O-2         1.400E+016    -1.610
1860.0
C5H11O2H-2+HO2<=>C5H11O2-2+H2O2                    2.400E+012     0.000
10000.0
C5H11O2H-2+O2<=>C5H11O2-2+HO2                      4.380E+013    -0.812
33640.0
C5H11O2-3+CH3O2=>O2+C5H11O-3+CH3O                 1.400E+016    -1.610
1860.0
C5H11O2-3+C5H11O2-3=>O2+C5H11O-3+C5H11O-3         1.400E+016    -1.610
1860.0
C5H11O2H-3+HO2<=>C5H11O2-3+H2O2                    2.400E+012     0.000
10000.0
C5H11O2H-3+O2<=>C5H11O2-3+HO2                      4.380E+013    -0.812
33640.0
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C5H11O2H-1<=>C5H11O-1+OH                          1.500E+016     0.000
42000.0
C5H11O2H-2<=>C5H11O-2+OH                          1.050E+016     0.000
41600.0
C5H11O2H-3<=>C5H11O-3+OH                          1.050E+016     0.000
41600.0
CH2O+PC4H9<=>C5H11O-1                             6.250E+010     0.000
11900.0
CH3CHO+NC3H7<=>C5H11O-2                           7.500E+010     0.000
11900.0
C2H5+C2H5CHO<=>C5H11O-3                           8.500E+010     0.000
11900.0

!REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
C5H11-1+O2<=>C5H11O2-1                            6.865E+016    -1.627
198.7
C5H11-2+O2<=>C5H11O2-2                            3.487E+014    -0.816
-536.5
C5H11-3+O2<=>C5H11O2-3                            3.487E+014    -0.816
-536.5

!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-
5701
C5H11O2-1<=>C5H10OOH1-2                           4.009E+08      1.100
30100.0
C5H11O2-1<=>C5H10OOH1-3                           1.360E+07      1.300
18200.0
C5H11O2-1<=>C5H10OOH1-4                           3.718E+06      1.200
16600.0
C5H11O2-1<=>C5H10OOH1-5                           2.941E+05      1.500
19900.0
C5H11O2-2<=>C5H10OOH2-1                           1.458E+09      1.100
33500.0
C5H11O2-2<=>C5H10OOH2-3                           1.716E+09      0.900
29500.0
C5H11O2-2<=>C5H10OOH2-4                           7.033E+10      0.200
18500.0
C5H11O2-2<=>C5H10OOH2-5                           1.233E+06      1.500
20000.0
C5H11O2-3<=>C5H10OOH3-1                           2.877E+07      1.400
20800.0
C5H11O2-3<=>C5H10OOH3-2                           3.432E+09      0.900
29500.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2011, 115, 13425-13442
C5H11O2-1<=>C5H10-1+HO2                           2.580E+007     1.580
28500.0
C5H11O2-2<=>C5H10-1+HO2                           2.403E+009     1.130
30100.0
C5H11O2-2<=>C5H10-2+HO2                           5.140E+009     1.010
29362.0
C5H11O2-3<=>C5H10-2+HO2                           7.200E+010     0.730
29883.0
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!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
C5H10OOH1-2<=>C5H10O1-2+OH                          7.340E+009     0.930
10900.0
C5H10OOH1-3<=>C5H10O1-3+OH                          8.450E+008     0.900
15300.0
C5H10OOH1-4<=>C5H10O1-4+OH                          4.820E+007     0.940
9000.0
C5H10OOH1-5<=>C5H10O1-5+OH                          2.890E+007     0.760
11300.0
C5H10OOH2-1<=>C5H10O1-2+OH                          1.160E+011     0.430
10700.0
C5H10OOH2-3<=>C5H10O2-3+OH                          4.435E+009     0.916
9389.0
C5H10OOH2-4<=>C5H10O2-4+OH                          2.413E+009     0.717
15402.0
C5H10OOH2-5<=>C5H10O1-4+OH                          2.480E+009     0.350
11200.0
C5H10OOH3-1<=>C5H10O1-3+OH                          2.030E+010     0.460
17700.0
C5H10OOH3-2<=>C5H10O2-3+OH                          1.336E+010     0.791
9583.0

C5H10O1-2+OH=>CH2CO+NC3H7+H2O                       2.500E+012     0.000
0.0
C5H10O1-3+OH=>C2H4+C2H5CO+H2O                       2.500E+012     0.000
0.0
C5H10O1-4+OH=>CH3COCH2+C2H4+H2O                     2.500E+012     0.000
0.0
C5H10O1-5+OH=>CH2CH2CHO+C2H4+H2O                    2.500E+012     0.000
0.0
C5H10O2-3+OH=>CH3CHCO+C2H5+H2O                      2.500E+012     0.000
0.0
C5H10O2-4+OH=>CH3CO+C3H6+H2O                        2.500E+012     0.000
0.0
C5H10O1-2+OH=>C2H3CHO+C2H5+H2O                      2.500E+012     0.000
0.0
C5H10O1-3+OH=>HCO+C4H8-1+H2O                        2.500E+012     0.000
0.0
C5H10O1-4+OH=>CH2CHO+C3H6+H2O                       2.500E+012     0.000
0.0
C5H10O1-5+OH=>CH2O+C4H71-3+H2O                      2.500E+012     0.000
0.0
C5H10O2-3+OH=>C2H3COCH3+CH3+H2O                     2.500E+012     0.000
0.0
C5H10O2-4+OH=>CH3CHO+C3H5-S+H2O                     2.500E+012     0.000
0.0
C5H10O1-2+HO2=>CH2CO+NC3H7+H2O2                     5.000E+012     0.000
17700.0
C5H10O1-3+HO2=>C2H4+C2H5CO+H2O2                     5.000E+012     0.000
17700.0
C5H10O1-4+HO2=>CH3COCH2+C2H4+H2O2                   5.000E+012     0.000
17700.0
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C5H10O1-5+HO2=>CH2CH2CHO+C2H4+H2O2                5.000E+012     0.000
17700.0
C5H10O2-3+HO2=>CH3CHCO+C2H5+H2O2                  5.000E+012     0.000
17700.0
C5H10O2-4+HO2=>CH3CO+C3H6+H2O2                    5.000E+012     0.000
17700.0
C5H10O1-2+HO2=>C2H3CHO+C2H5+H2O2                  5.000E+012     0.000
17700.0
C5H10O1-3+HO2=>HCO+C4H8-1+H2O2                    5.000E+012     0.000
17700.0
C5H10O1-4+HO2=>CH2CHO+C3H6+H2O2                   5.000E+012     0.000
17700.0
C5H10O1-5+HO2=>CH2O+C4H71-3+H2O2                  5.000E+012     0.000
17700.0
C5H10O2-3+HO2=>C2H3COCH3+CH3+H2O2                 5.000E+012     0.000
17700.0
C5H10O2-4+HO2=>CH3CHO+C3H5-S+H2O2                 5.000E+012     0.000
17700.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
C5H10OOH1-2<=>C5H10-1+HO2                          1.040E+010     0.940
15100.0
C5H10OOH2-1<=>C5H10-1+HO2                          2.210E+012     0.230
15600.0
C5H10OOH2-3<=>C5H10-2+HO2                          4.543E+010     0.751
15100.0
C5H10OOH3-2<=>C5H10-2+HO2                          4.066E+010     0.678
15034.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
C5H10OOH1-3=>OH+CH2O+C4H8-1                       9.100E+008     1.400
25500.0
C5H10OOH2-4=>OH+CH3CHO+C3H6                       1.180E+009     1.200
22700.0
C5H10OOH3-1=>OH+C2H5CHO+C2H4                      3.096E+018    -1.730
26820.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
C5H10OOH1-2=>C2H5+AC3H5OOH                        2.410E+010     1.020
28200.0
C5H10OOH2-5=>C2H4+C3H6OOH2-1                      6.860E+013     0.100
29000.0
C5H10OOH1-4=>C3H6+C2H4O2H                         5.080E+011     0.700
28700.0

!REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.55
C5H10OOH1-2+O2<=>C5H10OOH1-2O2                     1.918E+014    -0.816
-536.5
C5H10OOH1-3+O2<=>C5H10OOH1-3O2                     1.918E+014    -0.816
-536.5
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C5H10OOH1-4+O2<=>C5H10OOH1-4O2                    1.918E+014    -0.816
-536.5
C5H10OOH1-5+O2<=>C5H10OOH1-5O2                    3.776E+016    -1.627
198.7
C5H10OOH2-1+O2<=>C5H10OOH2-1O2                    3.776E+016    -1.627
198.7
C5H10OOH2-3+O2<=>C5H10OOH2-3O2                    1.918E+014    -0.816
-536.5
C5H10OOH2-4+O2<=>C5H10OOH2-4O2                    1.918E+014    -0.816
-536.5
C5H10OOH2-5+O2<=>C5H10OOH2-5O2                    3.776E+016    -1.627
198.7
C5H10OOH3-1+O2<=>C5H10OOH3-1O2                    3.776E+016    -1.627
198.7
C5H10OOH3-2+O2<=>C5H10OOH3-2O2                    1.918E+014    -0.816
-536.5

!"ALTERNATIVE" ISOMERISATIONS
C5H10OOH1-2O2<=>NC5KET12+OH                       2.441E+07      1.600
27900.0
C5H10OOH1-2O2<=>C5H93-1,2OOH                      1.716E+09      0.900
29500.0
C5H10OOH1-2O2<=>C5H92-4,5OOH                      7.033E+10      0.200
18500.0
C5H10OOH1-2O2<=>C5H91-4,5OOH                      1.233E+06      1.500
20000.0

C5H10OOH1-3O2<=>NC5KET13+OH                       1.098E+04      2.400
19900.0
C5H10OOH1-3O2<=>C5H92-1,3OOH                      3.432E+09      0.900
29500.0
C5H10OOH1-3O2<=>C5H92-3,5OOH                      3.432E+09      0.900
29500.0
C5H10OOH1-3O2<=>C5H91-3,5OOH                      2.877E+07      1.400
20800.0

C5H10OOH1-4O2<=>NC5KET14+OH                       1.256E+03      2.200
17400.0
C5H10OOH1-4O2<=>C5H92-1,4OOH                      7.033E+10      0.200
18500.0
C5H10OOH1-4O2<=>C5H93-1,4OOH                      1.716E+09      0.900
29500.0
C5H10OOH1-4O2<=>C5H91-2,5OOH                      1.458E+09      1.100
33500.0

C5H10OOH1-5O2<=>NC5KET15+OH                       1.115E+03      1.800
16600.0
C5H10OOH1-5O2<=>C5H92-1,5OOH                      3.718E+06      1.200
16600.0
DUP
C5H10OOH1-5O2<=>C5H93-1,5OOH                      1.360E+07      1.300
18200.0
C5H10OOH1-5O2<=>C5H92-1,5OOH                      4.009E+08      1.100
30100.0
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DUP

C5H10OOH2-1O2<=>NC5KET21+OH 2.763E+08 1.200
25700.0
C5H10OOH2-1O2<=>C5H93-1,2OOH 1.360E+07 1.300
18200.0
C5H10OOH2-1O2<=>C5H92-4,5OOH 3.718E+06 1.200
16600.0
C5H10OOH2-1O2<=>C5H91-4,5OOH 2.941E+05 1.500
19900.0

C5H10OOH2-3O2<=>NC5KET23+OH 1.748E+08 1.700
26000.0
C5H10OOH2-3O2<=>C5H91-2,3OOH 2.877E+07 1.400
20800.0
C5H10OOH2-3O2<=>C5H92-3,4OOH 3.432E+09 0.900
29500.0
C5H10OOH2-3O2<=>C5H91-3,4OOH 2.877E+07 1.400
20800.0

C5H10OOH2-4O2<=>NC5KET24+OH 1.754E+02 3.100
17500.0
C5H10OOH2-4O2<=>C5H91-2,4OOH 1.233E+06 1.500
20000.0
DUP
C5H10OOH2-4O2<=>C5H93-2,4OOH 1.716E+09 0.900
29500.0
C5H10OOH2-4O2<=>C5H91-2,4OOH 1.458E+09 1.100
33500.0
DUP

C5H10OOH2-5O2<=>NC5KET25+OH 3.768E+02 2.200
15300.0
C5H10OOH2-5O2<=>C5H91-2,5OOH 2.941E+05 1.500
19900.0
C5H10OOH2-5O2<=>C5H93-1,4OOH 1.360E+07 1.300
18200.0
C5H10OOH2-5O2<=>C5H92-1,4OOH 4.009E+08 1.100
30100.0

C5H10OOH3-1O2<=>NC5KET31+OH 5.786E+01 2.900
17000.0
C5H10OOH3-1O2<=>C5H92-1,3OOH 4.009E+08 1.100
30100.0
C5H10OOH3-1O2<=>C5H92-3,5OOH 3.718E+06 1.200
16600.0
C5H10OOH3-1O2<=>C5H91-3,5OOH 2.941E+05 1.500
19900.0

C5H10OOH3-2O2<=>NC5KET32+OH 1.748E+08 1.700
26000.0
C5H10OOH3-2O2<=>C5H91-2,3OOH 1.458E+09 1.100
33500.0

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C5H10OOH3-2O2<=>C5H92-3,4OOH                 7.033E+10      0.200
18500.0
C5H10OOH3-2O2<=>C5H91-3,4OOH                 1.233E+06      1.500
20000.0

C5H91-2,3OOH<=>C5H91-3OOH+HO2                2.210E+012     0.230
15600.0
C5H91-3OOH=>C2H5CHO+C2H3+OH                 1.050E+016     0.000
41600.0
C5H91-3OOH=>C2H3CHO+C2H5+OH                 1.050E+016     0.000
41600.0

C5H91-2,4OOH<=>C5H91-4OOH+HO2                2.210E+012     0.230
15600.0
C5H91-4OOH=>CH3CHO+C3H5-A+OH                1.050E+016     0.000
41600.0
C5H91-4OOH=>SC3H5CHO+CH3+OH                 1.050E+016     0.000
41600.0

C5H91-2,5OOH<=>C5H91-5OOH+HO2                2.210E+012     0.230
15600.0
C5H91-5OOH=>CH2O+C4H71-4+OH                 1.500E+016     0.000
42000.0

C5H91-3,4OOH=>C3KET12+C2H4+OH                3.096E+018    -1.730
26820.0

C5H91-3,5OOH=>C3KET13+C2H4+OH                3.096E+018    -1.730
26820.0

C5H91-4,5OOH=>AC3H5OOH+C2H4+HO2              6.860E+013     0.100
29000.0

C5H92-1,3OOH<=>C5H91-3OOH+HO2                 1.040E+010     0.940
15100.0
C5H92-1,3OOH<=>C5H92-1OOH+HO2                 4.066E+010     0.678
15034.0
C5H92-1OOH=>CH2O+C4H71-1+OH                 1.500E+016     0.000
42000.0

C5H92-1,4OOH<=>C5H91-4OOH+HO2                 1.040E+010     0.940
15100.0
C5H92-1,4OOH=>AC3H5OOH+CH3CHO+OH            2.410E+010     1.020
28200.0

C5H92-1,5OOH<=>C5H91-5OOH+HO2                 1.040E+010     0.940
15100.0
C5H92-1,5OOH<=>AC3H5OOH+C2H4O2H               2.410E+010     1.020
28200.0

C5H92-3,4OOH<=>C5H92-4OOH+HO2                 4.066E+010     0.678
15034.0
C5H92-4OOH=>CH3CHO+C3H5-S+OH                1.050E+016     0.000
41600.0
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C5H92-4OOH=>SC3H5CHO+CH3+OH                    1.050E+016     0.000
41600.0

C5H92-3,5OOH<=>C5H92-5OOH+HO2                   4.066E+010     0.678
15034.0
C5H92-5OOH=>CH2O+C4H71-3+OH                    1.500E+016     0.000
42000.0

C5H92-4,5OOH=>HO2CH2CHO+C3H6+OH                1.180E+009     1.200
22700.0

C5H93-1,2OOH<=>C5H92-1OOH+HO2                   4.543E+010     0.751
15100.0

C5H93-1,4OOH<=>C5H92-5OOH+HO2                   4.543E+010     0.751
15100.0
C5H93-1,4OOH=>CH2O+C4H71-3OOH+OH               9.100E+008     1.400
25500.0

C5H93-1,5OOH=>CH2O+C4H71-4OOH+OH               1.820E+009     1.400
25500.0

C5H93-2,4OOH<=>C5H92-4OOH+HO2                   9.086E+010     0.751
15100.0

!O2QOOH = CYCLIC ETHER + OH
C5H91-2,3OOH<=>C5H9O1-2OOH-3+OH                 1.160E+011     0.430
10700.0
C5H9O1-2OOH-3=>C2H5CHO+CH2CHO+OH                1.050E+016     0.000
41600.0

C5H91-2,3OOH<=>C5H9O1-3OOH-2+OH                 2.030E+010     0.460
17700.0
C5H9O1-3OOH-2=>C2H5CHO+CH2CHO+OH                1.050E+016     0.000
41600.0
C5H9O1-3OOH-2=>CH2O+C3H6CHO-3+OH                1.050E+016     0.000
41600.0

C5H91-2,4OOH<=>C5H9O1-2OOH-4+OH                 1.160E+011     0.430
10700.0
C5H9O1-2OOH-4=>CH3CHO+C3H5O+OH                  1.050E+016     0.000
41600.0

C5H91-2,4OOH<=>C5H9O1-4OOH-2+OH                 2.480E+009     0.350
11200.0
C5H9O1-4OOH-2=>CH2O+C3H6CHO-2+OH                1.050E+016     0.000
41600.0
C5H9O1-4OOH-2=>C3H6+OCH2CHO+OH                  1.050E+016     0.000
41600.0
OCH2CHO<=>CH2O+HCO                              2.900E+012     0.380
11080.0

C5H91-2,5OOH<=>C5H9O1-2OOH-5+OH                 1.160E+011     0.430
10700.0
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```
C5H9O1-2OOH-5<=>C5H9O1-2O-5+OH                    4.151E+019    -1.310
45700.0
C5H9O1-2O-5=>CH2O+CH2CHO+C2H4                     1.326E+021    -2.349
25084.0

C5H91-2,5OOH<=>C5H9O1-5OOH-2+OH                   2.890E+007     0.760
11300.0
C5H9O1-5OOH-2=>CH2O+C3H6CHO-1+OH                  1.050E+016     0.000
41600.0
C5H9O1-5OOH-2=>C2H4+CH2OCH2CHO+OH                 1.050E+016     0.000
41600.0
CH2OCH2CHO<=>CH2O+CH2CHO                          1.600E+013     0.000
25500.0

C5H91-3,4OOH<=>C5H9O1-3OOH-4+OH                   2.030E+010     0.460
17700.0
C5H9O1-3OOH-4=>CH3CHO+CH2CH2CHO+OH                1.050E+016     0.000
41600.0

C5H91-3,4OOH<=>C5H9O1-4OOH-3+OH                   2.480E+009     0.350
11200.0
C5H9O1-4OOH-3=>C2H4+C2H4OCHO+OH                   1.050E+016     0.000
41600.0
C2H4OCHO<=>CH3CHO+HCO                             2.900E+012     0.380
11080.0

C5H91-3,5OOH<=>C5H9O1-3OOH-5+OH                   2.030E+010     0.460
17700.0
C5H9O1-3OOH-5=>CH2O+C4H7O1-4+OH                   1.500E+016     0.000
42000.0
C4H7O1-4<=>CH2O+C3H5-A                            1.326E+021    -2.349
25084.0

C5H91-3,5OOH<=>C5H9O1-5OOH-3+OH                   2.890E+007     0.760
11300.0
C5H9O1-5OOH-3<=>CH2CH2OCH2CH2CHO+OH               1.050E+016     0.000
41600.0
CH2CH2OCH2CH2CHO=>CH2O+C2H4+CH2CHO                1.600E+013     0.000
25500.0

C5H91-4,5OOH<=>C5H9O1-4OOH-5+OH                   2.480E+009     0.350
11200.0
C5H9O1-4OOH-5=>CH2O+C3H6CHO-1+OH                  1.500E+016     0.000
42000.0

C5H91-4,5OOH<=>C5H9O1-5OOH-2+OH                   2.890E+007     0.760
11300.0

C5H92-1,3OOH<=>C5H9O1-2OOH-3+OH                   7.340E+009     0.930
10900.0

C5H92-1,3OOH<=>C5H9O2-3OOH-1+OH                   1.408E+010     0.784
9591.0
```

C5H9O2-3OOH-1=>CH2O+C3H6CHO-3+OH 1.500E+016 0.000
42000.0

C5H92-1,4OOH<=>C5H9O1-2OOH-4+OH 7.340E+009 0.930
10900.0

C5H92-1,4OOH<=>C5H9O2-4OOH-1+OH 2.680E+009 0.700
15415.0
C5H9O2-4OOH-1=>CH2O+C3H6CHO-2+OH 1.500E+016 0.000
42000.0

C5H92-1,5OOH<=>C5H9O1-2OOH-5+OH 7.340E+009 0.930
10900.0

C5H92-1,5OOH<=>C5H9O1-4OOH-5+OH 4.820E+007 0.940
9000.0

C5H92-3,4OOH<=>C5H9O2-3OOH-4+OH 1.408E+010 0.784
9591.0

C5H92-3,4OOH<=>C5H9O2-4OOH-3+OH 2.680E+009 0.700
15415.0
C5H9O2-4OOH-3=>CH3CHO+CH3CHCHO+OH 1.050E+016 0.000
41600.0

C5H92-3,5OOH<=>C5H9O2-3OOH-5+OH 1.408E+010 0.784
9591.0
C5H9O2-3OOH-5=>CH2O+C4H7O+OH 1.500E+016 0.000
42000.0

C5H92-3,5OOH<=>C5H9O1-4OOH-3+OH 4.820E+007 0.940
9000.0

C5H92-4,5OOH<=>C5H9O2-4OOH-1+OH 2.680E+009 0.700
15415.0

C5H92-4,5OOH<=>C5H9O1-4OOH-2+OH 4.820E+007 0.940
9000.0

C5H93-1,2OOH<=>C5H9O1-3OOH-2+OH 8.450E+008 0.900
15300.0

C5H93-1,2OOH<=>C5H9O2-3OOH-1+OH 4.881E+009 0.900
9403.0

C5H93-1,4OOH<=>C5H9O1-3OOH-4+OH 8.450E+008 0.900
15300.0

C5H93-1,4OOH<=>C5H9O2-3OOH-5+OH 4.881E+009 0.900
9403.0

C5H93-1,5OOH<=>C5H9O1-3OOH-5+OH 8.450E+008 0.900
15300.0

```
C5H93-2,4OOH<=>C5H9O2-3OOH-4+OH                    9.762E+009     0.900
9403.0

!CONCERTED ELIMINATIONS
C5H10OOH1-2O2<=>C5H92-1OOH+HO2                     5.140E+009     1.010
29362.0
C5H10OOH1-3O2<=>C5H92-1OOH+HO2                     3.600E+010     0.730
29883.0
C5H10OOH1-3O2<=>C5H92-5OOH+HO2                     3.600E+010     0.730
29883.0
C5H10OOH1-4O2<=>C5H91-5OOH+HO2                     2.403E+009     1.130
30100.0
C5H10OOH1-4O2<=>C5H92-5OOH+HO2                     5.140E+009     1.010
29362.0
C5H10OOH1-5O2<=>C5H91-5OOH+HO2                     2.580E+007     1.580
28500.0
C5H10OOH2-3O2<=>C5H92-4OOH+HO2                     3.600E+010     0.730
29883.0
C5H10OOH2-4O2<=>C5H92-4OOH+HO2                     5.140E+009     1.010
29362.0
C5H10OOH2-4O2<=>C5H91-4OOH+HO2                     2.403E+009     1.130
30100.0
C5H10OOH2-5O2<=>C5H91-4OOH+HO2                     2.580E+007     1.580
28500.0
C5H10OOH3-1O2<=>C5H91-3OOH+HO2                     2.580E+007     1.580
28500.0
C5H10OOH3-2O2<=>C5H91-3OOH+HO2                     2.403E+009     1.130
30100.0

NC5KET12<=>CHOC4H8O+OH                             1.050E+016     0.000
42600.0
CHOC4H8O<=>NC3H7CHO+HCO                            2.900E+012     0.380
11080.0

NC5KET13<=>CHOCH2C3H6O+OH                          1.050E+016     0.000
42600.0
CHOCH2C3H6O<=>C2H5CHO+CH2CHO                       2.900E+012     0.380
11080.0

NC5KET14<=>CHOCH2CH2C2H4O+OH                       1.050E+016     0.000
42600.0
CHOCH2CH2C2H4O<=>CH3CHO+CH2CH2CHO                  2.900E+012     0.380
11080.0

NC5KET15<=>CHOCH2CH2CH2CH2O+OH                     1.500E+016     0.000
43000.0
CHOCH2CH2CH2CH2O<=>CH2O+C3H6CHO-1                  2.900E+012     0.380
11080.0

NC5KET21<=>C3H7COCH2O+OH                           1.500E+016     0.000
43000.0
C3H7COCH2O<=>CH2O+NC3H7CO                          2.900E+012     0.380
11080.0
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```
NC5KET23<=>CH3COC3H6O+OH                           1.050E+016     0.000
42600.0
CH3COC3H6O<=>C2H5CHO+CH3CO                         2.900E+012     0.380
11080.0

NC5KET24<=>CH3COCH2C2H4O+OH                        1.050E+016     0.000
42600.0
CH3COCH2C2H4O<=>CH3CHO+CH3COCH2                    2.900E+012     0.380
11080.0

NC5KET25<=>CH3COCH2CH2CH2O+OH                      1.500E+016     0.000
43000.0
CH3COCH2CH2CH2O<=>CH2O+CH2CH2COCH3                 2.900E+012     0.380
11080.0

NC5KET31<=>C2H5COCH2CH2O+OH                        1.500E+016     0.000
43000.0
C2H5COCH2CH2O<=>C2H5COCH2+CH2O                     2.900E+012     0.380
11080.0

NC5KET32<=>C2H5COC2H4O+OH                          1.050E+016     0.000
42600.0
C2H5COC2H4O<=>CH3CHO+C2H5CO                        2.900E+012     0.380
11080.0

C5H10-1+OH<=>C5H10OH-1                             4.750E+012     0.000
-782.0
C5H10-2+OH<=>C5H10OH-2                             4.750E+012     0.000
-782.0
C5H10OH-1+O2<=>O2C5H10OH-1                         2.000E+012     0.000
0.0
O2C5H10OH-1=>NC3H7CHO+CH2O+OH                      2.500E+010     0.000
18860.0
C5H10OH-2+O2<=>O2C5H10OH-2                         2.000E+012     0.000
0.0
O2C5H10OH-2=>C2H5CHO+CH3CHO+OH                     2.500E+010     0.000
18860.0

!Pressure dependent unimolecular decomposition rate constants calculated
by JB 7/10/2013 based on LJ parameters from A. W. Jasper, J. A. Miller.
Combust. Flame (2013) for n-pentane
IC5H12 <=> IC3H7+C2H5 1.469E+026 -2.659 86860.0
PLOG  / 1.000E-002 4.070E+095 -23.37 121614. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E-001 2.800E+090 -21.55 122339. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+000 8.580E+079 -18.27 119001. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 3.960E+075 -16.97 117015. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 1.410E+069 -15.06 113723. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 7.290E+063 -13.51 110811. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
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PLOG  / 2.000E+001 2.460E+058 -11.91 107645. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 1.550E+051  -9.83 103292. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12 <=> SC4H9+CH3 8.694E+023 -2.019 87290.0
PLOG  / 1.000E-002 1.050E+093 -22.64 121641. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E-001 1.310E+088 -20.89 122563. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+000 6.800E+077 -17.67 119420. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 3.550E+073 -16.39 117484. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 1.430E+067 -14.49 114248. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 7.810E+061 -12.94 111365. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 2.700E+056 -11.35 108218. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 1.660E+049  -9.26 103871. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12 <=> IC4H9+CH3 1.067E+021 -1.460 89070.0
PLOG  / 1.000E-002 2.910E+088 -21.68 121666. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E-001 4.790E+084 -20.23 123421. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 1.000E+000 2.450E+075 -17.28 121108. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+000 2.210E+071 -16.05 119391. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 1.560E+065 -14.22 116397. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 1.120E+060 -12.70 113651. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 4.350E+054 -11.12 110591. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 2.490E+047  -9.02 106282. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12 <=> AC5H11+H 5.090E+017 -0.417 101180.0
PLOG  / 1.000E-002 8.010E+067 -16.14 118712. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 7%
PLOG  / 1.000E-001 1.480E+072 -16.92 125626. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E+000 7.250E+070 -16.14 129319. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+000 9.570E+068 -15.50 129394. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 5.000E+000 2.140E+065 -14.33 128592. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 4.960E+061 -13.21 127269. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
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PLOG  / 2.000E+001 2.300E+057 -11.91 125334. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 5.700E+050  -9.95 121933. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%

IC5H12 <=> BC5H11+H 6.342E+018 -0.784 96250.0
PLOG  / 1.000E-002 1.240E+077 -18.65 120361. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 6%
PLOG  / 1.000E-001 1.430E+078 -18.53 125424. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E+000 2.480E+073 -16.81 126657. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+000 3.390E+070 -15.90 125951. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 4.900E+065 -14.41 124153. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 1.950E+061 -13.09 122150. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 2.310E+056 -11.63 119644. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 2.030E+049  -9.56 115729. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12 <=> CC5H11+H 1.739E+018 -0.685 97930.0
PLOG  / 1.000E-002 7.610E+073 -17.85 119817. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 6%
PLOG  / 1.000E-001 1.220E+076 -18.05 125581. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E+000 3.070E+072 -16.65 127663. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+000 8.790E+069 -15.82 127218. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 3.060E+065 -14.44 125747. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 2.110E+061 -13.18 123961. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 2.000E+001 3.770E+056 -11.76 121634. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 4.400E+049  -9.73 117871. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12 <=> DC5H11+H 5.061E+017 -0.633 101180.0
PLOG  / 1.000E-002 7.960E+067 -16.35 118712. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 7%
PLOG  / 1.000E-001 1.480E+072 -17.13 125626. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 1.000E+000 7.210E+070 -16.36 129319. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+000 9.510E+068 -15.71 129394. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 5.000E+000 2.130E+065 -14.55 128592. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 1.000E+001 4.940E+061 -13.43 127269. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
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```
PLOG  / 2.000E+001 2.290E+057 -12.12 125334. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 5.660E+050 -10.17 121933. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%

IC5H12+H<=>AC5H11+H2 3.490E+05 2.690 6450.0
IC5H12+H<=>BC5H11+H2 6.020E+05 2.400 2583.0
IC5H12+H<=>CC5H11+H2 1.300E+06 2.400 4471.0
IC5H12+H<=>DC5H11+H2 1.745E+05 2.690 6450.0
IC5H12+O<=>AC5H11+OH 1.130E+14 0.000 7850.0
IC5H12+O<=>BC5H11+OH 3.968E+05 2.401 1150.0
IC5H12+O<=>CC5H11+OH 5.946E+05 2.439 2846.0
IC5H12+O<=>DC5H11+OH 1.046E+06 2.424 4766.0

IC5H12+OH<=>AC5H11+H2O 1.054E+010 0.970  1586.0
IC5H12+OH<=>BC5H11+H2O 5.730E+010 0.510    63.0
IC5H12+OH<=>CC5H11+H2O 4.670E+007 1.610   -35.0
IC5H12+OH<=>DC5H11+H2O 5.270E+009 0.970  1586.0

IC5H12+CH3<=>AC5H11+CH4 9.040E-01 3.650 7154.0
IC5H12+CH3<=>BC5H11+CH4 6.010E-10 6.360 893.0
IC5H12+CH3<=>CC5H11+CH4 8.400E+04 2.133 7574.0
IC5H12+CH3<=>DC5H11+CH4 4.520E-01 3.650 7154.0
IC5H12+HO2<=>AC5H11+H2O2 4.080E+01 3.590 17160.0
IC5H12+HO2<=>BC5H11+H2O2 6.504E+02 3.010 12090.0
IC5H12+HO2<=>CC5H11+H2O2 6.320E+01 3.370 13720.0
IC5H12+HO2<=>DC5H11+H2O2 2.040E+01 3.590 17160.0
IC5H12+CH3O2<=>AC5H11+CH3O2H 1.386E+00 3.970 18280.0
IC5H12+CH3O2<=>BC5H11+CH3O2H 2.620E+02 3.120 11100.0
IC5H12+CH3O2<=>CC5H11+CH3O2H 1.019E+01 3.580 14810.0
IC5H12+CH3O2<=>DC5H11+CH3O2H 6.930E-01 3.970 18280.0
IC5H12+CH3O<=>AC5H11+CH3OH 3.000E+11 0.000 7000.0
IC5H12+CH3O<=>BC5H11+CH3OH 1.900E+10 0.000 2800.0
IC5H12+CH3O<=>CC5H11+CH3OH 1.100E+11 0.000 5000.0
IC5H12+CH3O<=>DC5H11+CH3OH 1.500E+11 0.000 7000.0
IC5H12+O2<=>AC5H11+HO2 4.200E+13 0.000 52800.0
IC5H12+O2<=>BC5H11+HO2 7.000E+12 0.000 48000.0
IC5H12+O2<=>CC5H11+HO2 1.400E+13 0.000 50160.0
IC5H12+O2<=>DC5H11+HO2 2.100E+13 0.000 52800.0
IC5H12+C2H5<=>AC5H11+C2H6 1.000E+11 0.000 13400.0
IC5H12+C2H5<=>BC5H11+C2H6 1.000E+11 0.000 7900.0
IC5H12+C2H5<=>CC5H11+C2H6 5.000E+10 0.000 10400.0
IC5H12+C2H5<=>DC5H11+C2H6 5.000E+10 0.000 13400.0
IC5H12+C2H3<=>AC5H11+C2H4 1.000E+12 0.000 18000.0
IC5H12+C2H3<=>BC5H11+C2H4 2.000E+11 0.000 14300.0
IC5H12+C2H3<=>CC5H11+C2H4 4.000E+11 0.000 16800.0
IC5H12+C2H3<=>DC5H11+C2H4 5.000E+11 0.000 18000.0
IC5H12+AC5H11<=>BC5H11+IC5H12 2.500E+10 0.000 7900.0
IC5H12+AC5H11<=>CC5H11+IC5H12 5.000E+10 0.000 10400.0
IC5H12+AC5H11<=>DC5H11+IC5H12 7.500E+10 0.000 12300.0
IC5H12+BC5H11<=>CC5H11+IC5H12 5.000E+10 0.000 10400.0
IC5H12+BC5H11<=>DC5H11+IC5H12 7.500E+10 0.000 12300.0
IC5H12+CC5H11<=>DC5H11+IC5H12 7.500E+10 0.000 12300.0
IC5H12+O2CHO<=>AC5H11+HO2CHO 1.680E+13 0.000 20440.0
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```
IC5H12+O2CHO<=>BC5H11+HO2CHO 1.500E+04 2.500 12260.0
IC5H12+O2CHO<=>CC5H11+HO2CHO 5.600E+12 0.000 17690.0
IC5H12+O2CHO<=>DC5H11+HO2CHO 8.400E+12 0.000 20440.0

C3H6+C2H5<=>AC5H11  1.420E+03 2.670  6850.0
C4H8-1+CH3<=>AC5H11 1.890E+03 2.670  6850.0
AC5H10+H<=>AC5H11   6.250E+11 0.510  2620.0
AC5H11<=>DC5H11     3.000E+11 0.000 21100.0
IC4H8+CH3<=>BC5H11  4.400E+04 2.480  6130.0
AC5H10+H<=>BC5H11   1.060E+12 0.510  1230.0
BC5H10+H<=>BC5H11   6.250E+11 0.510  2620.0
C4H8-2+CH3<=>CC5H11 1.890E+03 2.670  6850.0
BC5H10+H<=>CC5H11   2.500E+11 0.510  2620.0
CC5H10+H<=>CC5H11   6.250E+11 0.510  2620.0
C2H4+IC3H7<=>DC5H11 8.800E+03 2.480  6130.0
CC5H10+H<=>DC5H11   2.500E+11 0.510  2620.0
!
!   correct A factors for c5h11+o2 reactions    CW2
!
!AC5H11+O2<=>AC5H10+HO2 2.000E-18 0.000 5000.0
!BC5H11+O2<=>AC5H10+HO2 2.000E-18 0.000 5000.0
!BC5H11+O2<=>BC5H10+HO2 2.000E-18 0.000 5000.0
!CC5H11+O2<=>BC5H10+HO2 2.000E-18 0.000 5000.0
AC5H11+O2<=>AC5H10+HO2 2.000E+12 0.000 5000.0
BC5H11+O2<=>AC5H10+HO2 2.000E+12 0.000 5000.0
BC5H11+O2<=>BC5H10+HO2 2.000E+12 0.000 5000.0
CC5H11+O2<=>BC5H10+HO2 2.000E+12 0.000 5000.0
!
! end of modications      CW2
!
CC5H11+O2<=>CC5H10+HO2 5.350E-01 3.710 9322.0
DC5H11+O2<=>CC5H10+HO2 8.370E-01 3.590 11960.0
AC5H11+HO2<=>AC5H11O+OH 9.000E+12 0.000 -1000.0
BC5H11+HO2<=>BC5H11O+OH 9.000E+12 0.000 -1000.0
CC5H11+HO2<=>CC5H11O+OH 9.000E+12 0.000 -1000.0
DC5H11+HO2<=>DC5H11O+OH 9.000E+12 0.000 -1000.0
AC5H11+CH3O2<=>AC5H11O+CH3O 9.000E+12 0.000 -1000.0
BC5H11+CH3O2<=>BC5H11O+CH3O 9.000E+12 0.000 -1000.0
CC5H11+CH3O2<=>CC5H11O+CH3O 9.000E+12 0.000 -1000.0
DC5H11+CH3O2<=>DC5H11O+CH3O 9.000E+12 0.000 -1000.0
!
AC5H10  =>  IC4H7+CH3 1.900E+20 -1.582 75930.0
!AC5H10<=>C3H5-T+C2H5 8.922E+24 -2.409 100500.0
!
BC5H10  =>  C4H72-2+CH3     8.900E+16  0.0  98262.0
!
!BC5H10<=>IC4H7+CH3 2.610E+19 -1.017 79020.0
BC5H10  =>  IC4H7+CH3 2.500E+17  0.00  96844.0
!
CC5H10  =>  C4H71-3+CH3 1.302E+21 -1.639 76140.0
!
! CW2 add unimolecular decomposition of ac5h10, bc5h10, cc5h10
!
AC5H10  => AC5H9-A2 + H   1.000E+15   0.0  84000.0
```

```
AC5H10  => AC5H9-C  + H   1.000E+15   0.0  84000.0
AC5H10  => AC5H9-D  + H   1.000E+15   0.0  84000.0
!
!  CW10   increase rates of these reactions for bc5h10
!
!BC5H10  =  AC5H9-C  + H   1.200E+15   0.0  84308.0
!    rev  /  8.300E+12  0.00  0.00  /
!BC5H10  =  CC5H9-B  + H   9.600E+14   0.0  83276.0
!    rev  /  8.300E+12  0.00  0.00  /
!
BC5H10  =  AC5H9-C  + H   2.400E+15   0.0  84308.0
    rev  /  1.660E+13  0.00  0.00  /
BC5H10  =  CC5H9-B  + H   1.920E+15   0.0  83276.0
    rev  /  1.660E+13  0.00  0.00  /
!
CC5H10  => CC5H9-A  + H   1.000E+15   0.0  84000.0
CC5H10  => CC5H9-B  + H   1.000E+15   0.0  84000.0
!
!  CW2 add fuel + O2 reactions for ac5h10, bc5h10, cc5h10
!
AC5H10 + O2 =>  AC5H9-A2 + HO2   2.100E+12  0.0  35000.
AC5H10 + O2 =>  AC5H9-C  + HO2   2.100E+12  0.0  30000.
AC5H10 + O2 =>  AC5H9-D  + HO2   2.100E+12  0.0  38000.
!
BC5H10 + O2 =>  AC5H9-C  + HO2   4.200E+12  0.0  35246.
BC5H10 + O2 =>  CC5H9-B  + HO2   2.100E+12  0.0  34314.
!
CC5H10 + O2 =>  CC5H9-A  + HO2   4.200E+12  0.00 35000.
CC5H10 + O2 =>  CC5H9-B  + HO2   2.100e+12  0.00 28000.
!
!   end of CW2 additions here
!
!AC5H10+OH<=>SC4H9+CH2O 2.000E+10 0.000 4000.0
BC5H10+OH<=>IC3H7+CH3CHO 2.000E+10 0.000 4000.0
CC5H10+OH<=>IC4H9+CH2O 2.000E+10 0.000 4000.0
!AC5H10+O<=>SC4H9+HCO 7.230E+05 2.340 -1050.0
!AC5H10+O<=>IC3H7+CH3CO 7.230E+05 2.340 -1050.0
!AC5H10+O<=>IC4H9+HCO 7.230E+05 2.340 -1050.0
!AC5H10+H<=>AC5H9-A2+H2 1.730E+05 2.500 2492.0
AC5H10+H<=>AC5H9-C+H2 3.376E+05 2.360 207.0
AC5H10+H<=>AC5H9-D+H2 1.950E+06 2.400 4471.0
!AC5H10+OH<=>AC5H9-A2+H2O 3.120E+06 2.000 -298.0
AC5H10+OH<=>AC5H9-C+H2O 2.764E+04 2.640 -1919.0
AC5H10+OH<=>AC5H9-D+H2O 7.010E+07 1.610 -35.0
!AC5H10+CH3<=>AC5H9-A2+CH4 2.210E+00 3.500 5675.0
AC5H10+CH3<=>AC5H9-C+CH4 3.690E+00 3.310 4002.0
AC5H10+CH3<=>AC5H9-D+CH4 2.270E+00 3.460 5481.0
AC5H10+HO2<=>AC5H9-A2+H2O2 9.639E+03 2.600 13910.0
AC5H10+HO2<=>AC5H9-C+H2O2 4.820E+03 2.550 10530.0
AC5H10+HO2<=>AC5H9-D+H2O2 1.450E+04 2.600 13910.0
AC5H10+CH3O2<=>AC5H9-A2+CH3O2H 9.639E+03 2.600 13910.0
AC5H10+CH3O2<=>AC5H9-C+CH3O2H 4.820E+03 2.550 10530.0
AC5H10+CH3O2<=>AC5H9-D+CH3O2H 1.450E+04 2.600 13910.0
AC5H10+CH3O<=>AC5H9-A2+CH3OH 9.000E+01 2.950 11990.0
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AC5H10+CH3O<=>AC5H9-C+CH3OH 4.000E+01 2.900 8609.0
AC5H10+CH3O<=>AC5H9-D+CH3OH 2.180E+11 0.000 4571.0
!
BC5H10+H<=>AC5H9-C+H2 3.500E+05 2.500 2510.0
BC5H10+H<=>CC5H9-B+H2 1.700E+05 2.500 2510.0
BC5H10+O<=>AC5H9-C+OH 2.600E+11 0.700 3250.0
BC5H10+O<=>CC5H9-B+OH 1.300E+11 0.700 3250.0
BC5H10+OH<=>AC5H9-C+H2O 6.000E+06 2.000 -298.0
BC5H10+OH<=>CC5H9-B+H2O 3.000E+06 2.000 -298.0
BC5H10+CH3<=>AC5H9-C+CH4 4.400E+00 3.500 5670.0
BC5H10+CH3<=>CC5H9-B+CH4 2.200E+00 3.500 5670.0
BC5H10+HO2<=>AC5H9-C+H2O2 1.900E+04 2.600 13900.0
BC5H10+HO2<=>CC5H9-B+H2O2 9.600E+03 2.600 13900.0
BC5H10+CH3O2<=>AC5H9-C+CH3O2H 4.000E+12   0.0  17050.
BC5H10+CH3O2<=>CC5H9-B+CH3O2H 2.000E+12   0.0  17050.
!
! BC5H10+CH3O<=>AC5H9-C+CH3OH   4.000E+12   0.0   4000.
! BC5H10+CH3O<=>CC5H9-B+CH3OH   2.000E+12   0.0   4000.
!
!   CW7  increase rate to increase methanol production
!
BC5H10+CH3O<=>AC5H9-C+CH3OH   2.000E+13   0.0   4000.
BC5H10+CH3O<=>CC5H9-B+CH3OH   1.000E+13   0.0   4000.
!
CC5H10+H<=>CC5H9-A+H2 3.900E+06 2.400 4471.0
CC5H10+H<=>CC5H9-B+H2 2.650E+06 2.200 0.0
CC5H10+OH<=>CC5H9-A+H2O 1.400E+08 1.610 -35.0
CC5H10+OH<=>CC5H9-B+H2O 6.140E+02 3.200 -3500.0
CC5H10+CH3<=>CC5H9-A+CH4 4.530E+00 3.460 5481.0
CC5H10+CH3<=>CC5H9-B+CH4 4.613E+00 3.100 2330.0
CC5H10+HO2<=>CC5H9-A+H2O2 2.892E+04 2.600 13910.0
CC5H10+HO2<=>CC5H9-B+H2O2 1.810E+03 2.500 7154.0
CC5H10+CH3O2<=>CC5H9-A+CH3O2H 4.000E+12   0.0  17050.
CC5H10+CH3O2<=>CC5H9-B+CH3O2H 2.000E+12   0.0  17050.
CC5H10+CH3O<=>CC5H9-A+CH3OH   4.000E+12   0.0  4000.
CC5H10+CH3O<=>CC5H9-B+CH3OH   2.000E+12   0.0  4000.
!
!     low temperature consumption of allyl radicals not in Glaude
mechanism
!
! AC5H9-A2+HO2<=>AC5H9O-A2+OH        9.640E+12 0.000 0.0
! AC5H9-A2+CH3O2<=>AC5H9O-A2+CH3O    9.640E+12 0.000 0.0
! AC5H9-A2+C2H5O2<=>AC5H9O-A2+C2H5O  9.640E+12 0.000 0.0
! AC5H9-C+HO2<=>AC5H9O-C+OH          9.640E+12 0.000 0.0
! AC5H9-C+CH3O2<=>AC5H9O-C+CH3O      9.640E+12 0.000 0.0
! AC5H9-C+C2H5O2<=>AC5H9O-C+C2H5O    9.640E+12 0.000 0.0
AC5H9-D<=>AC5H9-A2                 1.113E+12 0.000 31700.0
! CC5H9-B+HO2<=>CC5H9O-B+OH          9.640E+12 0.000 0.0
! CC5H9-B+CH3O2<=>CC5H9O-B+CH3O      9.640E+12 0.000 0.0
! CC5H9-B+C2H5O2<=>CC5H9O-B+C2H5O    9.640E+12 0.000 0.0
!
!AC5H9O-A2<=>C4H71-2+CH2O 9.210E+17 -1.430 30330.0
!AC5H9O-C<=>CH3CHO+C3H5-T 3.231E+22 -2.630 30310.0
!CC5H9O-B<=>CH3COCH3+C2H3 9.475E+18 -4.457 32000.0
```

```
!
!  include c5h9+o2 reaction pathways       CW2
!
!    Glaude R26 = AC5H9-C       Glaude  R27 = CC5H9-B
!    Glaude R36 = AC5H9-A2      Glaude  R45 = AC5H9-D
!
!
!   add Glaude reactions for c5h9 + ho2 = c5h9ooh = oh + c5h9o = products
!
!   increase formation of precursor for i2c4h7cho in PZ-3
!   code CW34, more in CW35, iterate for CW37
!
!   code 40, increase production of c5h9c-booh and therefore cc5h9o-b
!   code 40 produces NTC behavior, reduce rate back to CW37 value for
CW41
!
!   code 41 increase production of c5h9b-aooh, therefore bc5h9o-a
!
AC5H9-C  +  HO2  => C5H9B-AOOH    0.500E+14   -0.8  0.00   !  PZ-1
!AC5H9-C  +  HO2  => C5H9B-AOOH    1.000E+14   -0.8  0.00   !  PZ-1
AC5H9-C  +  HO2  => C5H9A-COOH    0.500E+14   -0.8  0.00   !  PZ-2
!AC5H9-C  +  HO2  => C5H9A-COOH    1.000E+14   -0.8  0.00   !  PZ-2
CC5H9-B  +  HO2  => C5H9B-DOOH    0.500E+14   -0.8  0.00   !  PZ-3
!CC5H9-B  +  HO2  => C5H9B-DOOH    2.000E+14   -0.8  0.00   !  PZ-3
!CC5H9-B  +  HO2  => C5H9B-DOOH    5.000E+14   -0.8  0.00   !  PZ-3
!CC5H9-B  +  HO2  => C5H9B-DOOH    3.500E+14   -0.8  0.00   !  PZ-3
!CC5H9-B  +  HO2  => C5H9B-DOOH    1.000E+14   -0.8  0.00   !  PZ-3
!CC5H9-B  +  HO2  => C5H9C-BOOH    0.500E+14   -0.8  0.00   !  PZ-4
CC5H9-B  +  HO2  => C5H9C-BOOH    1.000E+14   -0.8  0.00   !  PZ-4
!
C5H9B-AOOH  =>  OH  +  BC5H9O-A   5.000E+15    0.0  42500.0  ! RC5H9O-1
C5H9A-COOH  =>  OH  +  AC5H9O-C   5.000E+15    0.0  42500.0  ! RC5H9O-2
C5H9B-DOOH  =>  OH  +  BC5H9O-D   5.000E+15    0.0  42500.0  ! RC5H9O-3
C5H9C-BOOH  =>  OH  +  CC5H9O-B   5.000E+15    0.0  42500.0  ! RC5H9O-4
!
AC5H9-C  +  O2  =>  IC5H8 + HO2       1.400E+12  0.0  15500.
AC5H9-D  +  O2  =>  IC5H8 + HO2       1.400E+12  0.0  13500.
!
CC5H9-A  +  O2  =>  IC5H8 + HO2       1.400E+12  0.0  13500.
CC5H9-B  +  O2  =>  IC5H8 + HO2       2.700E+12  0.0  15500.
!
!  add unimolecular decompositions of c5h9 species   CW2
!
AC5H9-C   =>  H  +  IC5H8             1.500E+13  0.0  51500.
AC5H9-D   =>  H  +  IC5H8             3.200E+13  0.0  34800.
!
CC5H9-A   =>  H  +  IC5H8             1.500E+13  0.0  45000.
CC5H9-B   =>  H  +  IC5H8             3.000E+13  0.0  51500.
!
!    increase consumption of ic5h8 x 5   CW83
!IC5H8  +  OH  =>  CH2O + IC4H7         1.400E+12  0.00  -1040.
!IC5H8  +   H  =>  C2H4 + C3H5-S        1.000E+12  0.00   1000.
IC5H8  +  OH  =>  CH2O + IC4H7         7.000E+12  0.00  -1040.
IC5H8  +   H  =>  C2H4 + C3H5-S        5.000E+12  0.00   1000.
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!
!
!   next reaction already in NUI Galway mechanism above
!AC5H9-A2      =>  C3H4-A + C2H5        2.000E+13  0.00  50000.
AC5H9-C       =>  CH3 + C4H6           1.000E+13  0.00  50000.
!    A factor of 50000.  from Glaude seems low??
AC5H9-D       =>  C2H4 + C3H5-T        2.000E+13  0.00  34500.
!
CC5H9-A       =>  C3H6 + C2H3          1.000E+13  0.00  50000.
CC5H9-A       =>  CH3 + C4H6           1.000E+13  0.00  50000.
!
!   end of added reactions for     CW2
!
AC5H11O2+IC5H12<=>AC5H11O2H+AC5H11 1.210E+13 0.000 20430.0
BC5H11O2+IC5H12<=>BC5H11O2H+AC5H11 1.210E+13 0.000 20430.0
CC5H11O2+IC5H12<=>CC5H11O2H+AC5H11 1.210E+13 0.000 20430.0
DC5H11O2+IC5H12<=>DC5H11O2H+AC5H11 1.210E+13 0.000 20430.0
AC5H11O2+IC5H12<=>AC5H11O2H+BC5H11 2.016E+12 0.000 16000.0
BC5H11O2+IC5H12<=>BC5H11O2H+BC5H11 2.016E+12 0.000 16000.0
CC5H11O2+IC5H12<=>CC5H11O2H+BC5H11 2.016E+12 0.000 16000.0
DC5H11O2+IC5H12<=>DC5H11O2H+BC5H11 2.016E+12 0.000 16000.0
AC5H11O2+IC5H12<=>AC5H11O2H+CC5H11 4.032E+12 0.000 17700.0
BC5H11O2+IC5H12<=>BC5H11O2H+CC5H11 4.032E+12 0.000 17700.0
CC5H11O2+IC5H12<=>CC5H11O2H+CC5H11 4.032E+12 0.000 17700.0
DC5H11O2+IC5H12<=>DC5H11O2H+CC5H11 4.032E+12 0.000 17700.0
AC5H11O2+IC5H12<=>AC5H11O2H+DC5H11 6.048E+12 0.000 20430.0
BC5H11O2+IC5H12<=>BC5H11O2H+DC5H11 6.048E+12 0.000 20430.0
CC5H11O2+IC5H12<=>CC5H11O2H+DC5H11 6.048E+12 0.000 20430.0
DC5H11O2+IC5H12<=>DC5H11O2H+DC5H11 6.048E+12 0.000 20430.0
AC5H11+AC5H11O2<=>AC5H11O+AC5H11O 9.000E+12 0.000 -1000.0
AC5H11+BC5H11O2<=>AC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
AC5H11+CC5H11O2<=>AC5H11O+CC5H11O 9.000E+12 0.000 -1000.0
AC5H11+DC5H11O2<=>AC5H11O+DC5H11O 9.000E+12 0.000 -1000.0
BC5H11+AC5H11O2<=>BC5H11O+AC5H11O 9.000E+12 0.000 -1000.0
BC5H11+BC5H11O2<=>BC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
BC5H11+CC5H11O2<=>BC5H11O+CC5H11O 9.000E+12 0.000 -1000.0
BC5H11+DC5H11O2<=>BC5H11O+DC5H11O 9.000E+12 0.000 -1000.0
CC5H11+AC5H11O2<=>CC5H11O+AC5H11O 9.000E+12 0.000 -1000.0
CC5H11+BC5H11O2<=>CC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
CC5H11+CC5H11O2<=>CC5H11O+CC5H11O 9.000E+12 0.000 -1000.0
CC5H11+DC5H11O2<=>CC5H11O+DC5H11O 9.000E+12 0.000 -1000.0
DC5H11+AC5H11O2<=>DC5H11O+AC5H11O 9.000E+12 0.000 -1000.0
DC5H11+BC5H11O2<=>DC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
DC5H11+CC5H11O2<=>DC5H11O+CC5H11O 9.000E+12 0.000 -1000.0
DC5H11+DC5H11O2<=>DC5H11O+DC5H11O 9.000E+12 0.000 -1000.0
AC5H11O2+HO2<=>AC5H11O2H+O2 1.750E+10 0.000 -3275.0
AC5H11O2+H2O2<=>AC5H11O2H+HO2 2.400E+12 0.000 10000.0
AC5H11O2+AC5H11O2=>O2+AC5H11O+AC5H11O 1.400E+16 -1.610 1860.0
AC5H11O2+BC5H11O2=>O2+AC5H11O+BC5H11O 1.400E+16 -1.610 1860.0
AC5H11O2+CC5H11O2=>O2+AC5H11O+CC5H11O 1.400E+16 -1.610 1860.0
AC5H11O2+DC5H11O2=>O2+AC5H11O+DC5H11O 1.400E+16 -1.610 1860.0
AC5H11O2+CH3O2=>AC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0
BC5H11O2+HO2<=>BC5H11O2H+O2 1.750E+10 0.000 -3275.0
BC5H11O2+H2O2<=>BC5H11O2H+HO2 2.400E+12 0.000 10000.0
```

```
BC5H11O2+BC5H11O2=>O2+BC5H11O+BC5H11O 1.400E+16 -1.610 1860.0
BC5H11O2+CC5H11O2=>O2+BC5H11O+CC5H11O 1.400E+16 -1.610 1860.0
BC5H11O2+DC5H11O2=>O2+BC5H11O+DC5H11O 1.400E+16 -1.610 1860.0
BC5H11O2+CH3O2=>BC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0
CC5H11O2+HO2<=>CC5H11O2H+O2 1.750E+10 0.000 -3275.0
CC5H11O2+H2O2<=>CC5H11O2H+HO2 2.400E+12 0.000 10000.0
CC5H11O2+CC5H11O2=>O2+CC5H11O+CC5H11O 1.400E+16 -1.610 1860.0
CC5H11O2+DC5H11O2=>O2+CC5H11O+DC5H11O 1.400E+16 -1.610 1860.0
CC5H11O2+CH3O2=>CC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0
DC5H11O2+HO2<=>DC5H11O2H+O2 1.750E+10 -1.610 -3275.0
DC5H11O2+H2O2<=>DC5H11O2H+HO2 2.400E+12 0.000 10000.0
DC5H11O2+DC5H11O2=>O2+DC5H11O+DC5H11O 1.400E+16 -1.610 1860.0
DC5H11O2+CH3O2=>DC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0

AC5H11O2H<=>AC5H11O+OH 1.500E+16 0.000 42000.0
BC5H11O2H<=>BC5H11O+OH 6.000E+15 0.000 41200.0
CC5H11O2H<=>CC5H11O+OH 1.050E+16 0.000 41600.0
DC5H11O2H<=>DC5H11O+OH 1.500E+16 0.000 42000.0

CH2O+SC4H9<=>AC5H11O    6.250E+10 0.000 11900.0
C2H5+CH3COCH3<=>BC5H11O 8.500E+10 0.000 11900.0
CH3CHO+IC3H7<=>CC5H11O  7.500E+10 0.000 11900.0
CH2O+IC4H9<=>DC5H11O    6.250E+10 0.000 11900.0

!REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
AC5H11+O2<=>AC5H11O2   6.865E+016    -1.627     198.7
BC5H11+O2<=>BC5H11O2   9.756E+011     0.325    -417.3
CC5H11+O2<=>CC5H11O2   3.487E+014    -0.816    -536.5
DC5H11+O2<=>DC5H11O2   6.865E+016    -1.627     198.7

!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-
5701
AC5H11O2<=>AC5H10OOH-A 4.910E+07  1.300 21500.0
AC5H11O2<=>AC5H10OOH-B 2.309E+09  0.800 27100.0
AC5H11O2<=>AC5H10OOH-C 1.360E+07  1.300 18200.0
AC5H11O2<=>AC5H10OOH-D 1.233E+06  1.500 20000.0
BC5H11O2<=>BC5H10OOH-A 3.014E+09  1.200 33500.0
BC5H11O2<=>BC5H10OOH-C 6.513E+09  0.700 30100.0
BC5H11O2<=>BC5H10OOH-D 1.504E+08  1.100 21900.0
CC5H11O2<=>CC5H10OOH-A 2.877E+07  1.400 20800.0
CC5H11O2<=>CC5H10OOH-B 7.449E+09  0.600 27300.0
CC5H11O2<=>CC5H10OOH-D 1.458E+09  1.100 33500.0
DC5H11O2<=>DC5H10OOH-A 2.467E+06  1.500 20000.0
DC5H11O2<=>DC5H10OOH-B 1.231E+07  1.200 15400.0
DC5H11O2<=>DC5H10OOH-C 4.009E+08  1.100 30100.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2011, 115, 13425-13442
AC5H11O2<=>AC5H10+HO2  1.260E+08  1.320 28900.0
BC5H11O2<=>AC5H10+HO2  2.448E+10  0.890 29500.0
BC5H11O2<=>BC5H10+HO2  1.124E+11  0.580 29600.0
CC5H11O2<=>BC5H10+HO2  3.500E+10  0.710 30100.0
CC5H11O2<=>CC5H10+HO2  1.476E+09  1.210 29800.0
DC5H11O2<=>CC5H10+HO2  1.518E+07  1.660 28400.0
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!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
AC5H10OOH-A<=>A-AC5H10O+OH 4.100E+10 0.360 17200.0
AC5H10OOH-B<=>A-BC5H10O+OH 7.190E+09 0.880  9600.0
AC5H10OOH-C<=>A-CC5H10O+OH 1.701E+09 0.734 14983.0
AC5H10OOH-D<=>A-DC5H10O+OH 5.200E+08 0.670 10500.0
BC5H10OOH-A<=>A-BC5H10O+OH 1.050E+12 0.150  9600.0
BC5H10OOH-C<=>B-CC5H10O+OH 4.270E+10 0.520  8800.0
BC5H10OOH-D<=>B-DC5H10O+OH 1.030E+10 0.550 16200.0
CC5H10OOH-A<=>A-CC5H10O+OH 3.792E+07 1.517 16033.0
CC5H10OOH-B<=>B-CC5H10O+OH 5.360E+10 0.540  8900.0
CC5H10OOH-D<=>C-DC5H10O+OH 1.530E+10 0.640 10500.0
DC5H10OOH-A<=>A-DC5H10O+OH 5.200E+08 0.670 10500.0
DC5H10OOH-B<=>B-DC5H10O+OH 2.850E+08 0.920 13400.0
DC5H10OOH-C<=>C-DC5H10O+OH 1.120E+10 0.820 10900.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
AC5H10OOH-B<=>AC5H10+HO2 8.380E+09  0.920 14500.0
BC5H10OOH-A<=>AC5H10+HO2 3.890E+13 -0.150 15500.0
BC5H10OOH-C<=>BC5H10+HO2 3.010E+11  0.350 15200.0
CC5H10OOH-B<=>BC5H10+HO2 9.790E+12  0.040 15400.0
CC5H10OOH-D<=>CC5H10+HO2 6.830E+09  0.920 15100.0
DC5H10OOH-C<=>CC5H10+HO2 6.240E+10  0.720 15000.0

!REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS.
CHEM. A 2012, 116, 5068-5089
AC5H10OOH-C=>OH+CH2O+C4H8-2   1.960E+09 1.200 23400.0
AC5H10OOH-A=>OH+CH2O+C4H8-1   8.283E+13 -0.170 30090.0 !Not Villano Rates
BC5H10OOH-D=>OH+CH3COCH3+C2H4 1.182E+20 -2.060 24210.0 !Not Villano Rates
CC5H10OOH-A=>OH+CH3CHO+C3H6   3.530E+09 1.200 21900.0
DC5H10OOH-B=>OH+CH2O+IC4H8    6.270E+08 1.400 23600.0

!REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.65
AC5H10OOH-A+O2<=>AC5H10OOH-AO2  4.462E+16    -1.627     198.7
AC5H10OOH-B+O2<=>AC5H10OOH-BO2  6.341E+11     0.325    -417.3
AC5H10OOH-C+O2<=>AC5H10OOH-CO2  2.267E+14    -0.816    -536.5
AC5H10OOH-D+O2<=>AC5H10OOH-DO2  4.462E+16    -1.627     198.7
BC5H10OOH-A+O2<=>BC5H10OOH-AO2  4.462E+16    -1.627     198.7
BC5H10OOH-C+O2<=>BC5H10OOH-CO2  2.267E+14    -0.816    -536.5
BC5H10OOH-D+O2<=>BC5H10OOH-DO2  4.462E+16    -1.627     198.7
CC5H10OOH-A+O2<=>CC5H10OOH-AO2  4.462E+16    -1.627     198.7
CC5H10OOH-B+O2<=>CC5H10OOH-BO2  6.341E+11     0.325    -417.3
CC5H10OOH-D+O2<=>CC5H10OOH-DO2  4.462E+16    -1.627     198.7
DC5H10OOH-A+O2<=>DC5H10OOH-AO2  4.462E+16    -1.627     198.7
DC5H10OOH-B+O2<=>DC5H10OOH-BO2  6.341E+11     0.325    -417.3
DC5H10OOH-C+O2<=>DC5H10OOH-CO2  2.267E+14    -0.816    -536.5

!REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-
5701
AC5H10OOH-AO2<=>IC5KETAA+OH  5.188E+04 1.900 18800.0
AC5H10OOH-AO2<=>C5H9B-A,AOOH 2.309E+09 0.800 27100.0
AC5H10OOH-AO2<=>C5H9C-A,AOOH 1.360E+07 1.300 18200.0
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AC5H10OOH-AO2<=>C5H9D-A,AOOH 1.233E+06 1.500 20000.0

AC5H10OOH-BO2<=>IC5KETAB+OH  2.441E+07 1.600 27900.0
AC5H10OOH-BO2<=>C5H9A-A,BOOH 3.014E+09 1.200 33500.0
AC5H10OOH-BO2<=>C5H9C-A,BOOH 6.513E+09 0.700 30100.0
AC5H10OOH-BO2<=>C5H9D-A,BOOH 1.504E+08 1.100 21900.0

AC5H10OOH-CO2<=>IC5KETAC+OH  1.098E+04 2.400 19900.0
AC5H10OOH-CO2<=>C5H9A-A,COOH 2.877E+07 1.400 20800.0
AC5H10OOH-CO2<=>C5H9B-A,COOH 7.449E+09 0.600 27300.0
AC5H10OOH-CO2<=>C5H9D-A,COOH 1.458E+09 1.100 33500.0

AC5H10OOH-DO2<=>IC5KETAD+OH  4.766E+03 1.700 16600.0
AC5H10OOH-DO2<=>C5H9A-A,DOOH 2.467E+06 1.500 20000.0
AC5H10OOH-DO2<=>C5H9B-A,DOOH 1.231E+07 1.200 15400.0
AC5H10OOH-DO2<=>C5H9C-A,DOOH 4.009E+08 1.100 30100.0

BC5H10OOH-AO2<=>C5H9A-A,BOOH 4.910E+07 1.300 21500.0
BC5H10OOH-AO2<=>C5H9C-A,BOOH 1.360E+07 1.300 18200.0
BC5H10OOH-AO2<=>C5H9D-A,BOOH 1.233E+06 1.500 20000.0

BC5H10OOH-CO2<=>C5H9A-B,COOH 2.877E+07 1.400 20800.0
BC5H10OOH-CO2<=>C5H9D-B,COOH 1.458E+09 1.100 33500.0

BC5H10OOH-DO2<=>C5H9A-B,DOOH 2.467E+06 1.500 20000.0
BC5H10OOH-DO2<=>C5H9C-B,DOOH 4.009E+08 1.100 30100.0

CC5H10OOH-AO2<=>IC5KETCA+OH  5.786E+01 2.900 17000.0
CC5H10OOH-AO2<=>C5H9A-A,COOH 4.910E+07 1.300 21500.0
CC5H10OOH-AO2<=>C5H9B-A,COOH 2.309E+09 0.800 27100.0
CC5H10OOH-AO2<=>C5H9D-A,COOH 1.233E+06 1.500 20000.0

CC5H10OOH-BO2<=>IC5KETCB+OH  1.747E+08 1.700 26000.0
CC5H10OOH-BO2<=>C5H9A-B,COOH 3.014E+09 1.200 33500.0
CC5H10OOH-BO2<=>C5H9D-B,COOH 1.504E+08 1.100 21900.0

CC5H10OOH-DO2<=>IC5KETCD+OH  2.763E+08 1.200 25700.0
CC5H10OOH-DO2<=>C5H9A-C,DOOH 2.467E+06 1.500 20000.0
CC5H10OOH-DO2<=>C5H9B-C,DOOH 1.231E+07 1.200 15400.0

DC5H10OOH-AO2<=>IC5KETDA+OH  4.766E+03 1.700 16600.0
DC5H10OOH-AO2<=>C5H9A-A,DOOH 4.910E+07 1.300 21500.0
DC5H10OOH-AO2<=>C5H9B-A,DOOH 2.309E+09 0.800 27100.0
DC5H10OOH-AO2<=>C5H9C-A,DOOH 1.360E+07 1.300 18200.0
!
DC5H10OOH-BO2<=>IC5KETDB+OH  1.098E+04 2.400 19900.0
DC5H10OOH-BO2<=>C5H9A-B,DOOH 3.014E+09 1.200 33500.0
DC5H10OOH-BO2<=>C5H9C-B,DOOH 6.513E+09 0.700 30100.0
!
DC5H10OOH-CO2<=>IC5KETDC+OH  2.441E+07 1.600 27900.0
DC5H10OOH-CO2<=>C5H9A-C,DOOH 2.877E+07 1.400 20800.0
DC5H10OOH-CO2<=>C5H9B-C,DOOH 7.449E+09 0.600 27300.0
!
C5H9A-A,BOOH<=>C5H9A-AOOH+HO2 3.890E+13 -0.150 15500.0
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C5H9A-AOOH=>CH2O+C4H71-2+OH 1.500E+16 0.000 43000.0
!
C5H9A-A,COOH=>AC4H7OOH+CH2O+OH 1.978E+08 1.521 21890.0
!
C5H9A-A,DOOH<=>AC3H5OOH+C2H4O2H 1.978E+08 1.521 21890.0
!
C5H9A-B,COOH<=>C5H9A-COOH+HO2 3.890E+13 -0.150 15500.0
C5H9A-COOH=>CH3CHO+C3H5-T+OH 1.050E+16 0.000 42600.0
!
C5H9A-B,DOOH<=>C5H9A-DOOH+HO2 3.890E+13 -0.150 15500.0
C5H9A-DOOH=>CH2O+IC4H7+OH 1.500E+16 0.000 43000.0
!
C5H9A-C,DOOH=>C3H6+HO2CH2CHO+OH 3.530E+09 1.200 21900.0
!
C5H9B-A,AOOH<=>C5H9A-AOOH+HO2 1.676E+10  0.920 14500.0
!
C5H9B-A,COOH<=>C5H9A-COOH+HO2 8.380E+09  0.920 14500.0
C5H9B-A,COOH<=>C5H9B-AOOH+HO2 9.790E+12  0.040 15400.0
!
!   PZ-1, 2, 3, and 4
!
!
!    IC4H7CHO    2-methyl-2-butenal
!    IC3H5COCH3  3-methyl-3-buten-2-one
!    SC3H5CHO    methacrolein
!    I2C4H7CHO   3-methyl-2-butenal
!
!
!BC5H9O-A  =>  H + IC4H7CHO           1.100E+13   0.00   18400.0
!BC5H9O-A  =>  H + IC4H7CHO           6.000E+12   0.00   18400.0
BC5H9O-A  =>  H + IC4H7CHO           5.000E+12   0.00   18400.0
!BC5H9O-A  =>  H + IC4H7CHO           2.200E+13   0.00   18400.0
!BC5H9O-A  =>  H + IC4H7CHO           5.500E+13   0.00   18400.0
!BC5H9O-A  =>  H + IC4H7CHO           2.000E+14   0.00   18400.0
BC5H9O-A  =>  CH2O + C4H72-2         6.600E+13   0.00   22600.0
!BC5H9O-A  =>  CH2O + C4H72-2         1.320E+14   0.00   22600.0
BC5H9O-A + O2  =>  HO2 + IC4H7CHO    9.000E+09   0.00     400.0
!BC5H9O-A + O2  =>  HO2 + IC4H7CHO    1.800E+10   0.00     400.0
!
AC5H9O-C  =>  H + IC3H5COCH3         9.800E+12   0.00   17200.0
!AC5H9O-C  =>  H + IC3H5COCH3         1.960E+13   0.00   17200.0
!AC5H9O-C  =>  CH3 + SC3H5CHO         2.700E+13   0.00   12090.0
!AC5H9O-C  =>  CH3 + SC3H5CHO         5.400E+13   0.00   12090.0
AC5H9O-C  =>  CH3 + SC3H5CHO         1.500E+14   0.00   12090.0
AC5H9O-C  =>  CH3CHO + C3H5-T        3.400E+13   0.00   20410.0
!AC5H9O-C  =>  CH3CHO + C3H5-T        6.800E+13   0.00   20410.0
AC5H9O-C + O2  =>  HO2 + IC3H5COCH3  3.400E+13   0.00   20410.0
!AC5H9O-C + O2  =>  HO2 + IC3H5COCH3  6.800E+13   0.00   20410.0
!
!BC5H9O-D  =>  H + I2C4H7CHO          1.100E+13   0.00   18400.0
!BC5H9O-D  =>  H + I2C4H7CHO          4.500E+13   0.00   18400.0
BC5H9O-D  =>  H + I2C4H7CHO          9.000E+13   0.00   18400.0
!BC5H9O-D  =>  H + I2C4H7CHO          2.200E+13   0.00   18400.0
BC5H9O-D  =>  CH2O + C4H71-1         6.600E+13   0.00   22600.0
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```
BC5H9O-D + O2 =>  HO2 + I2C4H7CHO     9.900E+09   0.00     400.0
!
!CC5H9O-B  =>  CH3 + C2H3COCH3         5.400E+13   0.00   12090.0
CC5H9O-B  =>  CH3 + C2H3COCH3         1.080E+14   0.00   12090.0
!CC5H9O-B  =>  C2H3 + CH3COCH3         1.700E+14   0.00   20410.0
!CC5H9O-B  =>  C2H3 + CH3COCH3         3.400E+14   0.00   20410.0
!
!
!    c4h6oay is the same as sc3h5cho
!
!C4H6OAY + H => H2 + C2H3 + CH2CO             4.0E+0013  0.000  4200.0  !
ADZ 1034
!C4H6OAY + OH => H2O + C2H3 + CH2CO           4.0E+0012  0.000   500.0  !
ADZ 1035
!C4H6OAY + HO2 => H2O2 + C2H3 + CH2CO         1.0E+0012  0.000 10000.0  !
ADZ 1036
!C4H6OAY + CH3 => CH4 + C2H3 + CH2CO          2.0E-0006  0.000  2500.0  !
ADZ 1037
!C4H6OAY + C2H5 => C2H6 + C2H3 + CH2CO        1.3E+0012  0.000  8500.0  !
ADZ 1038
IC4H7CHO + H => H2 + C3H5-A + CH2CO          4.0E+0013  0.000  4200.0  !
ADZ 1039
!  the following reaction is also included in Galway mech above, but with
a much faster rate
!  keep this reaction rate and set of products and remove the other
version
IC4H7CHO + OH => H2O + C3H5-A + CH2CO        4.0E+0012  0.000   500.0  !
ADZ 1040
IC4H7CHO + HO2 => H2O2 + C3H5-A + CH2CO      1.0E+0012  0.000 10000.0  !
ADZ 1041
IC4H7CHO + CH3 => CH4 + C3H5-A + CH2CO       2.0E-0006  0.000  2500.0  !
ADZ 1042
IC4H7CHO + C2H5 => C2H6 + C3H5-A + CH2CO     1.3E+0012  0.000  8500.0  !
ADZ 1043
!I2C4H7CHO + H => H2 +      C3H5-A + CH2CO    4.0E+0013  0.000  4200.0  !
ADZ 1039
!I2C4H7CHO + OH => H2O +    C3H5-A + CH2CO    4.0E+0012  0.000   500.0  !
ADZ 1040
!I2C4H7CHO + HO2 => H2O2 +  C3H5-A + CH2CO    1.0E+0012  0.000 10000.0  !
ADZ 1041
!I2C4H7CHO + CH3 => CH4 +   C3H5-A + CH2CO    2.0E-0006  0.000  2500.0  !
ADZ 1042
!I2C4H7CHO + C2H5 => C2H6 + C3H5-A + CH2CO    1.3E+0012  0.000  8500.0  !
ADZ 1043
!
!I2C4H7CHO + H => H2 +      C3H5-A + CH2CO    8.0E+0012  0.000  4200.0  !
ADZ 1039
!I2C4H7CHO + OH => H2O +    C3H5-A + CH2CO    8.0E+0011  0.000   500.0  !
ADZ 1040
!I2C4H7CHO + HO2 => H2O2 +  C3H5-A + CH2CO    2.0E+0011  0.000 10000.0  !
ADZ 1041
!I2C4H7CHO + CH3 => CH4 +   C3H5-A + CH2CO    2.0E-0006  0.000  2500.0  !
ADZ 1042
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!I2C4H7CHO + C2H5 => C2H6 + C3H5-A + CH2CO    2.6E+0011  0.000  8500.0  !
ADZ 1043
!
I2C4H7CHO + H => H2 +      C3H5-A + CH2CO    4.0E+0012  0.000  4200.0  !
ADZ 1039
I2C4H7CHO + OH => H2O +    C3H5-A + CH2CO    4.0E+0011  0.000   500.0  !
ADZ 1040
I2C4H7CHO + HO2 => H2O2 +  C3H5-A + CH2CO    1.0E+0011  0.000 10000.0  !
ADZ 1041
I2C4H7CHO + CH3 => CH4 +   C3H5-A + CH2CO    1.0E-0006  0.000  2500.0  !
ADZ 1042
I2C4H7CHO + C2H5 => C2H6 + C3H5-A + CH2CO    1.3E+0011  0.000  8500.0  !
ADZ 1043
!
!C5H9B-AOOH=>CH2O+C4H72-2+OH 1.500E+16 0.000 43000.0
!
C5H9B-A,DOOH<=>C5H9A-DOOH+HO2 8.380E+09  0.920 14500.0
!
C5H9B-C,DOOH<=>C5H9B-DOOH+HO2 9.790E+12  0.040 15400.0
C5H9B-DOOH=>CH2O+IC4H7+OH 1.500E+16 0.000 43000.0

C5H9C-A,AOOH=>C4H72-1OOH+CH2O+OH 1.960E+09 1.200 23400.0

C5H9C-A,BOOH<=>C5H9B-AOOH+HO2 3.010E+11  0.350 15200.0

C5H9C-A,DOOH<=>C5H9C-AOOH+HO2 6.240E+10  0.720 15000.0
C5H9C-AOOH=>CH2O+C4H71-3+OH 1.500E+16 0.000 43000.0

C5H9C-B,DOOH<=>C5H9B-DOOH+HO2 3.010E+11  0.350 15200.0
C5H9C-B,DOOH<=>C5H9C-BOOH+HO2 6.240E+10  0.720 15000.0
C5H9C-BOOH=>CH3COCH3+C2H3+OH 6.000E+15 0.000 42200.0

C5H9D-A,AOOH=>AC3H5OOH+C2H4+HO2 1.978E+08 1.521 21890.0

C5H9D-A,BOOH=>TC3H5OOH+C2H4+HO2 1.960E+09 1.200 23400.0
TC3H5OOH=>CH2CO+CH3+OH 1.050E+16 0.000 42600.0

C5H9D-A,COOH<=>C5H9C-AOOH+HO2 6.830E+09  0.920 15100.0

C5H9D-B,COOH<=>C5H9C-BOOH+HO2 6.830E+09  0.920 15100.0

!O2QOOH = CYCLIC ETHER +OH
C5H9A-A,BOOH<=>C5H9OA-AOOH-B+OH 4.100E+10 0.360 17200.0
C5H9OA-AOOH-B=>CH2O+C2H5COCH2+OH 6.000E+15 0.000 42200.0

C5H9A-A,BOOH<=>C5H9OA-BOOH-A+OH 1.050E+12 0.150  9600.0
C5H9OA-BOOH-A=>CH2O+C2H5COCH2+OH 1.500E+16 0.000 43000.0

C5H9A-A,COOH<=>C5H9OA-AOOH-C+OH 4.100E+10 0.360 17200.0
C5H9OA-AOOH-C=>CH3CHO+C3H5O+OH 1.050E+16 0.000 42600.0

C5H9A-A,COOH<=>C5H9OA-COOH-A+OH 3.792E+07 1.517 16033.0
C5H9OA-COOH-A=>CH2O+C4H7O+OH 1.500E+16 0.000 43000.0
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C5H9A-A,DOOH<=>C5H9OA-AOOH-D+OH 4.100E+10 0.360 17200.0
C5H9OA-AOOH-D=>CH2O+CC3H5OCH2+OH 1.500E+16 0.000 43000.0
CC3H5OCH2<=>CH2O+C3H5-A 1.000E+14 0.000 25000.0

C5H9A-A,DOOH<=>C5H9OA-DOOH-A+OH 5.200E+08 0.670 10500.0
C5H9OA-DOOH-A=>CH2O+C4H7O1-4+OH 1.500E+16 0.000 43000.0

C5H9A-B,COOH<=>C5H9OA-BOOH-C+OH 1.050E+12 0.150  9600.0
C5H9OA-BOOH-C=>CH3CHO+CH3COCH2+OH 1.050E+16 0.000 42600.0

C5H9A-B,COOH<=>C5H9OA-COOH-B+OH 3.792E+07 1.517 16033.0
C5H9OA-COOH-B=>CH3CHO+CH3COCH2+OH 6.000E+15 0.000 42200.0

C5H9A-B,DOOH<=>C5H9OA-BOOH-D+OH 1.050E+12 0.150  9600.0
C5H9OA-BOOH-D=>CH2O+IC4H7O+OH 1.500E+16 0.000 43000.0

C5H9A-B,DOOH<=>C5H9OA-DOOH-B+OH 5.200E+08 0.670 10500.0
C5H9OA-DOOH-B<=>CH3COCH2OCH2CH2+OH 6.000E+15 0.000 42200.0
CH3COCH2OCH2CH2=>CH2O+C2H4+CH3CO 1.600E+13 0.000 25500.0

C5H9A-C,DOOH<=>C5H9OA-COOH-D+OH 3.792E+07 1.517 16033.0
C5H9OA-COOH-D=>CH2O+IC3H6CHO+OH 1.500E+16 0.000 43000.0

C5H9A-C,DOOH<=>C5H9OA-DOOH-C+OH 5.200E+08 0.670 10500.0
C5H9OA-DOOH-C=>CH2O+IC3H6CHO+OH 1.050E+16 0.000 42600.0

C5H9B-A,AOOH<=>C5H9OA-BOOH-A+OH 7.190E+09 0.880  9600.0
C5H9B-A,COOH<=>C5H9OA-BOOH-C+OH 7.190E+09 0.880  9600.0

C5H9B-A,COOH<=>C5H9OB-COOH-A+OH 5.360E+10 0.540  8900.0
C5H9OB-COOH-A=>CH2O+CH3CHCOCH3+OH 1.500E+16 0.000 43000.0

C5H9B-A,DOOH<=>C5H9OA-BOOH-D+OH 7.190E+09 0.880  9600.0

C5H9B-A,DOOH<=>C5H9OB-DOOH-A+OH 2.850E+08 0.920 13400.0
C5H9OB-DOOH-A=>CH2O+CH2CH2COCH3+OH 1.500E+16 0.000 43000.0

C5H9B-C,DOOH<=>C5H9OB-COOH-D+OH 5.360E+10 0.540  8900.0
C5H9OB-COOH-D=>CH2O+TC3H6CHO+OH 1.500E+16 0.000 43000.0

C5H9B-C,DOOH<=>C5H9OB-DOOH-C+OH 2.850E+08 0.920 13400.0
C5H9OB-DOOH-C=>CH3COCH3+CH2CHO+OH 1.050E+16 0.000 42600.0

C5H9C-A,AOOH<=>C5H9OA-COOH-A+OH 1.701E+09 0.734 14983.0
C5H9C-A,BOOH<=>C5H9OA-COOH-B+OH 1.701E+09 0.734 14983.0
C5H9C-A,BOOH<=>C5H9OB-COOH-A+OH 4.270E+10 0.520  8800.0
C5H9C-A,DOOH<=>C5H9OA-COOH-D+OH 1.701E+09 0.734 14983.0

C5H9C-A,DOOH<=>C5H9OC-DOOH-A+OH 1.120E+10 0.820 10900.0
C5H9OC-DOOH-A=>CH2O+C4H7O2-1+OH 1.500E+16 0.000 43000.0
C4H7O2-1<=>CH2O+C3H5-S 7.940E+14 0.000 19000.0

C5H9C-B,DOOH<=>C5H9OB-COOH-D+OH 4.270E+10 0.520  8800.0
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C5H9C-B,DOOH<=>C5H9OC-DOOH-B+OH 1.120E+10 0.820 10900.0
C5H9OC-DOOH-B=>CH3COCH3+CH2CHO+OH 6.000E+15 0.000 42200.0

C5H9D-A,AOOH<=>C5H9OA-DOOH-A+OH 5.200E+08 0.670 10500.0
C5H9D-A,BOOH<=>C5H9OA-DOOH-B+OH 5.200E+08 0.670 10500.0
C5H9D-A,BOOH<=>C5H9OB-DOOH-A+OH 1.030E+10 0.550 16200.0
C5H9D-A,COOH<=>C5H9OA-DOOH-C+OH 5.200E+08 0.670 10500.0
C5H9D-A,COOH<=>C5H9OC-DOOH-A+OH 1.530E+10 0.640 10500.0
C5H9D-B,COOH<=>C5H9OB-DOOH-C+OH 1.030E+10 0.550 16200.0
C5H9D-B,COOH<=>C5H9OC-DOOH-B+OH 1.530E+10 0.640 10500.0

!CONCERTED ELIMINATIONS
AC5H10OOH-AO2<=>C5H9A-AOOH+HO2 1.260E+08  1.320 28900.0
AC5H10OOH-BO2<=>C5H9A-AOOH+HO2 2.448E+10  0.890 29500.0
AC5H10OOH-BO2<=>C5H9B-AOOH+HO2 1.124E+11  0.580 29600.0
AC5H10OOH-CO2<=>C5H9B-AOOH+HO2 3.500E+10  0.710 30100.0
AC5H10OOH-CO2<=>C5H9C-AOOH+HO2 1.476E+09  1.210 29800.0
AC5H10OOH-DO2<=>C5H9C-AOOH+HO2 1.518E+07  1.660 28400.0
BC5H10OOH-CO2<=>C5H9C-BOOH+HO2 1.476E+09  1.210 29800.0
BC5H10OOH-DO2<=>C5H9C-BOOH+HO2 1.518E+07  1.660 28400.0
CC5H10OOH-AO2<=>C5H9A-COOH+HO2 1.260E+08  1.320 28900.0
CC5H10OOH-BO2<=>C5H9A-COOH+HO2 2.448E+10  0.890 29500.0
DC5H10OOH-AO2<=>C5H9A-DOOH+HO2 1.260E+08  1.320 28900.0
DC5H10OOH-BO2<=>C5H9A-DOOH+HO2 2.448E+10  0.890 29500.0
DC5H10OOH-BO2<=>C5H9B-DOOH+HO2 1.124E+11  0.580 29600.0
DC5H10OOH-CO2<=>C5H9B-DOOH+HO2 3.500E+10  0.710 30100.0

IC5KETAA<=>C2H5CH(CH2O)CHO+OH      1.500E+16 0.000 42000.0
C2H5CH(CH2O)CHO<=>CH2O+C3H6CHO-3   2.900E+12 0.380 11080.0

IC5KETAB<=>C3H5O(CH3)CHO+OH        6.000E+15 0.000 41200.0
C3H5O(CH3)CHO<=>C2H5COCH3+HCO      2.900E+12 0.380 11080.0

IC5KETAC<=>C2H4OCH(CH3)CHO+OH      1.050E+16 0.000 41600.0
C2H4OCH(CH3)CHO<=>CH3CHO+CH3CHCHO  2.900E+12 0.380 11080.0

IC5KETAD<=>CH2OC3H6CHO+OH          1.500E+16 0.000 42000.0
CH2OC3H6CHO<=>CH2O+IC3H6CHO        2.900E+12 0.380 11080.0

IC5KETCA<=>CH3COCH(CH3)CH2O+OH     1.500E+16 0.000 42000.0
CH3COCH(CH3)CH2O<=>CH2O+CH3CHCOCH3 2.900E+12 0.380 11080.0

IC5KETCB<=>CH3CO(CH3)C2H3O+OH      6.000E+15 0.000 41200.0
CH3CO(CH3)C2H3O<=>CH3COCH3+CH3CO   2.900E+12 0.380 11080.0

IC5KETCD<=>CH2OCOCH(CH3)CH3+OH     1.500E+16 0.000 42000.0
CH2OCOCH(CH3)CH3<=>CH2O+IC3H7CO    2.900E+12 0.380 11080.0

IC5KETDA<=>CHOC3H6CH2O+OH          1.500E+16 0.000 42000.0
CHOC3H6CH2O<=>CH2O+C3H6CHO-2       2.900E+12 0.380 11080.0

IC5KETDB<=>CHOCH2(CH3)C2H3O+OH     6.000E+15 0.000 41200.0
CHOCH2(CH3)C2H3O<=>CH3COCH3+CH2CHO 2.900E+12 0.380 11080.0
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IC5KETDC<=>CHOCHOCH(CH3)CH3+OH     1.050E+16 0.000 41600.0
CHOCHOCH(CH3)CH3<=>IC3H7CHO+HCO    2.900E+12 0.380 11080.0

A-AC5H10O+OH=>CH2O+C4H71-2+H2O 2.500E+12 0.000 0.0
A-BC5H10O+OH=>IC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0
A-CC5H10O+OH=>C3H6+CH3CO+H2O 2.500E+12 0.000 0.0
A-DC5H10O+OH=>C3H6+CH2CHO+H2O 2.500E+12 0.000 0.0
!
!  reduce production of ic3h5coch3 from b-cc5h10o
!
!B-CC5H10O+OH=>IC3H5COCH3+H+H2O 2.500E+12 0.000 0.0
B-CC5H10O+OH=>IC3H5COCH3+H+H2O 8.000E+11 0.000 0.0
!
B-DC5H10O+OH=>IC4H8+HCO+H2O 2.500E+12 0.000 0.0
C-DC5H10O+OH=>CH2CO+IC3H7+H2O 2.500E+12 0.000 0.0
A-AC5H10O+OH=>C2H3CHO+C2H5+H2O 2.500E+12 0.000 0.0
A-BC5H10O+OH=>CH2O+C4H72-2+H2O 2.500E+12 0.000 0.0
A-CC5H10O+OH=>C3H5-T+CH3CHO+H2O 2.500E+12 0.000 0.0
A-DC5H10O+OH=>CH3CHCHO+C2H4+H2O 2.500E+12 0.000 0.0
B-CC5H10O+OH=>IC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0
B-DC5H10O+OH=>CH3COCH3+C2H3+H2O 2.500E+12 0.000 0.0
C-DC5H10O+OH=>SC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0
A-AC5H10O+HO2=>CH2O+C4H71-2+H2O2 5.000E+12 0.000 17700.0
A-BC5H10O+HO2=>IC3H5CHO+CH3+H2O2 5.000E+12 0.000 17700.0
A-CC5H10O+HO2=>C3H6+CH3CO+H2O2 5.000E+12 0.000 17700.0
A-DC5H10O+HO2=>C3H6+CH2CHO+H2O2 5.000E+12 0.000 17700.0
B-CC5H10O+HO2=>IC3H5COCH3+H+H2O2 5.000E+12 0.000 17700.0
B-DC5H10O+HO2=>IC4H8+HCO+H2O2 5.000E+12 0.000 17700.0
C-DC5H10O+HO2=>CH2CO+IC3H7+H2O2 5.000E+12 0.000 17700.0
A-AC5H10O+HO2=>C2H3CHO+C2H5+H2O2 5.000E+12 0.000 17700.0
A-BC5H10O+HO2=>CH2O+C4H72-2+H2O2 5.000E+12 0.000 17700.0
A-CC5H10O+HO2=>C3H5-T+CH3CHO+H2O2 5.000E+12 0.000 17700.0
A-DC5H10O+HO2=>CH3CHCHO+C2H4+H2O2 5.000E+12 0.000 17700.0
B-CC5H10O+HO2=>IC3H5CHO+CH3+H2O2 5.000E+12 0.000 17700.0
B-DC5H10O+HO2=>CH3COCH3+C2H3+H2O2 5.000E+12 0.000 17700.0
C-DC5H10O+HO2=>SC3H5CHO+CH3+H2O2 5.000E+12 0.000 17700.0
!
!
!   CW31   increase oh addition pathways
!   CW32   increase oh addition pathways slightly less
!   CW33   optimize for ch3cho
!
!AC5H10+OH<=>AC5H10OH 1.000E+12 0.000 -1042.0
!AC5H10+OH<=>AC5H10OH 5.000E+12 0.000 -1042.0
!AC5H10+OH<=>AC5H10OH 3.000E+12 0.000 -1042.0
AC5H10+OH<=>AC5H10OH 4.000E+12 0.000 -1042.0
AC5H10OH+O2<=>AO2C5H10OH 2.000E+12 0.000 0.0
AO2C5H10OH=>C2H5COCH3+CH2O+OH 2.500E+10 0.000 18860.0
!
!   speed up following cycle of reactions to increase production of
ch3cho
!
!BC5H10+OH<=>BC5H10OH 1.000E+12 0.000 -1042.0
!BC5H10+OH<=>BC5H10OH 5.000E+12 0.000 -1042.0
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!BC5H10+OH<=>BC5H10OH 3.000E+12 0.000 -1042.0
!BC5H10+OH<=>BC5H10OH 4.000E+12 0.000 -1042.0
!  CW79   reduce rate of bc5h10+oh
!BC5H10+OH<=>BC5H10OH 4.000E+12 0.000      0.0
!    CW82   further reduce reaction of bc5h10+oh
BC5H10+OH<=>BC5H10OH 2.000E+12 0.000      0.0
!   CW8
!BC5H10+OH<=>BC5H10OH 3.000E+12 0.000 -1042.0
!
!BC5H10+OH<=>BC5H10OH 6.000E+12 0.000 -1042.0
!
BC5H10OH+O2<=>BO2C5H10OH 2.000E+12 0.000 0.0
BO2C5H10OH=>CH3COCH3+CH3CHO+OH 2.500E+10 0.000 18860.0
!
!
!CC5H10+OH<=>CC5H10OH 1.000E+12 0.000 -1042.0
!CC5H10+OH<=>CC5H10OH 5.000E+12 0.000 -1042.0
!CC5H10+OH<=>CC5H10OH 3.000E+12 0.000 -1042.0
CC5H10+OH<=>CC5H10OH 4.000E+12 0.000 -1042.0
CC5H10OH+O2<=>CO2C5H10OH 2.000E+12 0.000 0.0
CO2C5H10OH=>IC3H7CHO+CH2O+OH 2.500E+10 0.000 18860.0
!
!
CH3CHCHO+H2<=>C2H5CHO+H 2.160E+05 2.380 18990.0
!
!  increase consumption of ic3h5coch3 to match JSR results
!
IC3H5COCH3<=>IC3H5CO+CH3 2.200E+17 -0.510 75220.0
IC3H5COCH3<=>C3H5-T+CH3CO 6.070E+24 -2.210 96960.0
!
!IC3H5COCH3+OH<=>IC3H5COCH2+H2O 5.100E+11 0.000 1192.0
!IC3H5COCH3+O<=>IC3H5COCH2+OH 5.000E+12 0.000 5962.0
!IC3H5COCH3+H<=>IC3H5COCH2+H2 9.300E+12 0.000 6357.0
!IC3H5COCH3+CH3<=>IC3H5COCH2+CH4 1.620E+11 0.000 9630.0
!IC3H5COCH3+HO2<=>IC3H5COCH2+H2O2 8.500E+12 0.000 20460.0
!IC3H5COCH3+O2<=>IC3H5COCH2+HO2 6.000E+13 0.000 46000.0
!IC3H5COCH2<=>C3H5-T+CH2CO 5.972E+14 0.188 51272.0
!
!IC3H5COCH3+OH<=>AC3H4COCH3+H2O 3.120E+06 2.000 -298.0
!IC3H5COCH3+O<=>AC3H4COCH3+OH 6.030E+10 0.700 7633.0
!IC3H5COCH3+H<=>AC3H4COCH3+H2 1.730E+05 2.500 2492.0
!IC3H5COCH3+CH3<=>AC3H4COCH3+CH4 2.210E+00 3.500 5675.0
!IC3H5COCH3+HO2<=>AC3H4COCH3+H2O2 9.640E+03 2.600 13910.0
!IC3H5COCH3+O2<=>AC3H4COCH3+HO2 6.030E+13 0.000 47590.0
AC3H4COCH3<=>C3H4-A+CH3CO 1.400E+13 0.000 60000.0
!
IC3H5COCH3+OH<=>IC3H5COCH2+H2O 1.000E+12 0.000 1192.0
IC3H5COCH3+O<=>IC3H5COCH2+OH 1.000E+13 0.000 5962.0
IC3H5COCH3+H<=>IC3H5COCH2+H2 1.800E+13 0.000 6357.0
IC3H5COCH3+CH3<=>IC3H5COCH2+CH4 3.220E+11 0.000 9630.0
IC3H5COCH3+HO2<=>IC3H5COCH2+H2O2 1.700E+13 0.000 20460.0
IC3H5COCH3+O2 =>IC3H5COCH2+HO2 1.200E+14 0.000 46000.0
!
IC3H5COCH3+OH<=>AC3H4COCH3+H2O 6.120E+06 2.000 -298.0
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IC3H5COCH3+O<=>AC3H4COCH3+OH 1.230E+11 0.700 7633.0
IC3H5COCH3+H<=>AC3H4COCH3+H2 3.430E+05 2.500 2492.0
IC3H5COCH3+CH3<=>AC3H4COCH3+CH4 4.410E+00 3.500 5675.0
IC3H5COCH3+HO2<=>AC3H4COCH3+H2O2 1.940E+04 2.600 13910.0
IC3H5COCH3+O2 =>AC3H4COCH3+HO2 1.230E+14 0.000 47590.0
!
!Pressure dependent unimolecular decomposition rate constants calculated
by JB 7/10/2013 based on LJ parameters from A. W. Jasper, J. A. Miller.
Combust. Flame (2013) for n-pentane
NEOC5H12 <=> TC4H9+CH3 1.665E+30 -3.733 88230.0
PLOG  / 1.000E-002 3.250E+078 -18.54 107427. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 6%
PLOG  / 1.000E-001 8.690E+075 -17.45 109860. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E+000 4.530E+069 -15.35 109497. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+000 7.600E+066 -14.49 108643. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+000 4.020E+062 -13.18 106951. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%
PLOG  / 1.000E+001 9.500E+058 -12.10 105276. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%
PLOG  / 2.000E+001 1.300E+055 -10.95 103321. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%
PLOG  / 5.000E+001 7.340E+049  -9.41 100451. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%

NEOC5H12 <=> NEOC5H11+H 1.045E+19 -0.648 101180.0
PLOG  / 1.000E-002 2.570E+046  -9.94 102612. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 8%
PLOG  / 1.000E-001 8.980E+050 -10.81 109641. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 7%
PLOG  / 1.000E+000 1.010E+052 -10.71 114764. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 2.000E+000 2.350E+051 -10.42 115648. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG  / 5.000E+000 5.540E+049  -9.83 116204. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG  / 1.000E+001 7.900E+047  -9.21 116115. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG  / 2.000E+001 3.410E+045  -8.46 115568. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG  / 5.000E+001 4.840E+041  -7.28 114151. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NEOC5H12+H<=>NEOC5H11+H2              6.980E+05 2.690  6450.0
NEOC5H12+O<=>NEOC5H11+OH              2.260E+14 0.000  7850.0
NEOC5H12+OH<=>NEOC5H11+H2O            2.108E+10 0.970  1586.0
NEOC5H12+CH3<=>NEOC5H11+CH4           1.808E+00 3.650  7154.0
NEOC5H12+HO2<=>NEOC5H11+H2O2          8.160E+01 3.590 17160.0
NEOC5H12+CH3O<=>NEOC5H11+CH3OH        6.000E+11 0.000  7000.0
NEOC5H12+O2<=>NEOC5H11+HO2            8.400E+13 0.000 52800.0
NEOC5H12+C2H5<=>NEOC5H11+C2H6         2.000E+11 0.000 13400.0
NEOC5H12+C2H3<=>NEOC5H11+C2H4         2.000E+12 0.000 18000.0
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NEOC5H12+O2CHO<=>NEOC5H11+HO2CHO      2.772E+00 3.970 18280.0
NEOC5H12+CH3O2<=>NEOC5H11+CH3O2H      2.772E+00 3.970 18280.0

IC4H6OH+NEOC5H12<=>IC4H7OH+NEOC5H11   9.400E+02 3.300 19840.0
IC4H7O+NEOC5H12<=>IC4H7OH+NEOC5H11    5.400E+11 0.000  4000.0
TC3H6CHO+NEOC5H12<=>IC3H7CHO+NEOC5H11 9.400E+02 3.300 19840.0
NEOC5H12+CH2CCH2OH<=>NEOC5H11+C3H5OH  1.590E+12 0.000 20500.0

!REF:H. J. Curran Int. J. Chem. Kin. 2006, 38, 4, 250-275
IC4H8+CH3<=>NEOC5H11                  1.300E+03 2.480  8520.0

NEOC5H11+HO2<=>NEOC5H11O+OH           9.000E+12 0.000 -1000.0
NEOC5H11+CH3O2<=>NEOC5H11O+CH3O       9.000E+12 0.000 -1000.0

!REF:A. Miyoshi. Int. J. Chem. Kin. 2012, 44, 1, 59-74
NEOC5H11+O2<=>NEOC5H11O2               6.865E+16 -1.627 198.7

NEOC5H11O2+NEOC5H12<=>NEOC5H11O2H+NEOC5H11     2.419E+13  0.000 20430.0
NEOC5H11+NEOC5H11O2<=>NEOC5H11O+NEOC5H11O      9.000E+12  0.000 -1000.0
NEOC5H11O2+HO2<=>NEOC5H11O2H+O2                1.750E+10  0.000 -3275.0
NEOC5H11O2+H2O2<=>NEOC5H11O2H+HO2              2.400E+12  0.000 10000.0
NEOC5H11O2+CH3O2=>NEOC5H11O+CH3O+O2            1.400E+16 -1.610  1860.0
NEOC5H11O2+NEOC5H11O2=>O2+NEOC5H11O+NEOC5H11O  1.400E+16 -1.610  1860.0

NEOC5H11O2H<=>NEOC5H11O+OH         1.500E+016 0.000 42000.0

!REF:H. J. Curran Int. J. Chem. Kin. 2006, 38, 4, 250-275
CH2O+TC4H9<=>NEOC5H11O              5.000E+10 0.000  2330.0

!REF:S. Sharma, S. Raman, W. H. Green. J. Phys. Chem. A 2010, 114, 5689-
5701
NEOC5H11O2<=>NEOC5H10OOH            1.198E+09 1.200 21600.0

!REF:S. M. Villano, L. K. Huynh, H. -H. Carstensen, A. M. Dean. J. Phys.
Chem. A 2012, 116, 5068-5089
NEOC5H10OOH<=>NEO-C5H10O+OH         3.710E+09 0.700 15900.0

!REF:S. M. Villano, L. K. Huynh, H. -H. Carstensen, A. M. Dean. J. Phys.
Chem. A 2012, 116, 5068-5089
NEOC5H10OOH=>OH+CH2O+IC4H8          3.640E+09 1.300 23700.0
NEOC5H10OOH<=>IC4H7OOH+CH3          1.640E+07 2.000 28300.0

!REF:A. Miyoshi. Int. J. Chem. Kin. 2012, 44, 1, 59-74 !A*0.5
NEOC5H10OOH+O2<=>NEOC5H10OOH-O2     3.433E+16 -1.627  198.7

!REF:Analogy to 1st isomerisation
NEOC5H10OOH-O2<=>NEOC5H9Q2          7.987E+08 1.200 21600.0

!REF:Sharma iso-c5h12 analogy
NEOC5H10OOH-O2<=>NEOC5KET+OH        5.188E+04 1.900 18800.0

!REF:Analogy to B-scission of QOOH
NEOC5H9Q2<=>IC4H7OOH+CH2O2H        3.640E+09  1.300 23700.0
NEOC5H9Q2<=>IC4H6Q2-II+CH3         1.640E+07  2.000 28300.0
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!REF:Analogy to QOOH
NEOC5H9Q2<=>NEOC5H9O-OOH+OH          3.710E+09 0.700 15900.0

NEOC5KET<=>NEOC5KETOX+OH            1.500E+16  0.000 43000.0
NEOC5KETOX<=>TC3H6CHO+CH2O          2.475E+21 -2.540 15830.0
NEOC5KETOX<=>NEOC5KEJOL             1.203E+09  1.199 13600.7
NEOC5KEJOL<=>IC4H8OH+CO             2.273E+21 -2.340 11020.0
IC4H6Q2-II=>C3H4-A+CH2O+HO2+OH      1.000E+16  0.000 43000.0
NEOC5H9O-OOH=>C3H5-T+CH2O+CH2O+OH   1.000E+16  0.000 43000.0

NEO-C5H10O+OH<=>TC4H8CHO+H2O         2.500E+12 0.000     0.0
NEO-C5H10O+OH=>IC4H7+CH2O+H2O        2.500E+12 0.000     0.0
NEO-C5H10O+HO2<=>TC4H8CHO+H2O2       5.000E+12 0.000 17700.0
NEO-C5H10O+HO2=>IC4H7+CH2O+H2O2      5.000E+12 0.000 17700.0
NEO-C5H10O+H<=>TC4H8CHO+H2           3.544E+07 2.000  5000.0
NEO-C5H10O+H=>IC4H7+CH2O+H2          1.330E+06 2.540  6756.0
NEO-C5H10O<=>IC4H8+CH2O              3.800E+15 0.000 60700.0
END
!-------------------------------------------------------------------------
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