

!!
!!
!!
!!
!!!!
!!!!
!!!!
!!!!
!!!! Experimental and kinetic modeling study of the pyrolysis and
oxidation of diethylamine !!!
!!!!
!!!!
!!!! Cato A.R. Pappijn, Nicolas Vin, Florence H. Vermeire, Ruben Van de
Vijver, !!!
!!!! Olivier Herbinet, Frédérique Battin-Leclerc, Marie-Françoise
Reyniers, Guy B. Marin, !!!
!!!! Kevin M. Van Geem
!!!!
!!!!
!!!!
!!!! e-mail: kevin.vangeem@ugent.be
!!!!
!!!!
!!!!
!!!!
!!
!!
!!
!!

ELEMENTS
H C He AR O N HE
END

SPECIES
C3H8 !! InChI=1S/C3H8/c1-3-2/h3H2,1-2H3
C2H4Nr_Olef!! InChI=1S/C2H4N/c1-2-3/h1-2H,3H2/b2-1-
C2H4Nr_Olef_1 !! InChI=1S/C2H4N/c1-2-3/h1-2H,3H2/b2-1+
C2H5N !! InChI=1S/C2H5N/c1-2-3/h2-3H,1H3/b3-2+
C2H5N_1 !! InChI=1S/C2H5N/c1-2-3/h2-3H,1H3/b3-2-
C3H2Nr_Olef!! InChI=1S/C3H2N/c1-2-3-4/h1H2
C3H2Nr_Olef_1 !! InChI=1S/C3H2N/c1-2-3-4/h1-2H/b2-1-
C3H2Nr_Olef_2 !! InChI=1S/C3H2N/c1-2-3-4/h1-2H/b2-1+
C3H4Nr !! InChI=1S/C3H4N/c1-2-3-4/h1-2H2
C3H4Nr_1 !! InChI=1S/C3H4N/c1-2-3-4/h2H,1H
C3H4Nr_Olef!! InChI=1S/C3H4N/c1-3-4-2/h1,3H,2H2/b3-1+
C3H4Nr_Olef_1 !! InChI=1S/C3H4N/c1-3-4-2/h1,3H,2H2/b3-1-
C3H4Nr_Olef_2 !! InChI=1S/C3H4N/c1-3-4-2/h2-3H,1H2
C3H4Nr_Olef_3 !! InChI=1S/C3H4Nhr+CH3r=/c1-3-4-2/h1-2H2
C3H5N_Olef !! InChI=1S/C3H5N/c1-3-4-2/h3H,1-2H2
C3H5r_Olef !! InChI=1S/C3H5/c1-3-2/h3H,1-2H2
C3H5r_Olef_1 !! InChI=1S/C3H5/c1-3-2/h1H2,2H3
C3H5r_Olef_2 !! InChI=1S/C3H5/c1-3-2/h1,3H,2H3/b3-1+
C3H5r_Olef_3 !! InChI=1S/C3H5/c1-3-2/h1,3H,2H3/b3-1-
C3H6Nr !! InChI=1S/C3H6N/c1-2-3-4/h4H,2H2,1H3

C3H6Nr_1 !! InChI=1S/C3H6N/c1-3-4-2/h3H,1H2,2H3
C3H6Nr_2 !! InChI=1S/C3H6N/c1-3-4-2/h1-2H3
C3H6Nr_3 !! InChI=1S/C3H6N/c1-3-4-2/h1-3H2
C3H6Nr_4 !! InChI=1S/C3H6N/c1-3-4-2/h2H,3H2,1H3
C3H6Nr_Olef!! InChI=1S/C3H6N/c1-3-4-2/h1,3-4H,2H3/b3-1+
C3H6Nr_Olef_1 !! InChI=1S/C3H6N/c1-3-4-2/h1,3-4H,2H3/b3-1-
C3H6Nr_Olef_2 !! InChI=1S/C3H6N/c1-3-4-2/h3-4H,1-2H2
C3H6Nr_Olef_3 !! InChI=1S/C3H6N/c1-3-4-2/h4H,1H2,2H3
C3H6_Olef !! InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3
C3H7N !! InChI=1S/C3H7N/c1-3-4-2/h3H,1-2H3/b4-3+
C3H7N_1 !! InChI=1S/C3H7N/c1-3-4-2/h3H,1-2H3/b4-3-
C3H7N_2 !! InChI=1S/C3H7N/c1-3-4-2/h2-3H2,1H3
C3H7N_Olef !! InChI=1S/C3H7N/c1-3-4-2/h3-4H,1H2,2H3
C3H7r !! InChI=1S/C3H7/c1-3-2/h1,3H2,2H3
C3H7r_1 !! InChI=1S/C3H7/c1-3-2/h3H,1-2H3
C3H8Nr !! InChI=1S/C3H8N/c1-3-4-2/h3-4H,1-2H3
C3H8Nr_1 !! InChI=1S/C3H8N/c1-3-4-2/h4H,1,3H2,2H3
C3H8Nr_2 !! InChI=1S/C3H8N/c1-3-4-2/h4H,2-3H2,1H3
C4H4Nr_Olef!! InChI=1S/C4H4N/c1-4(2)3-5/h1H,2H3/b4-1-
C4H4Nr_Olef_1 !! InChI=1S/C4H4N/c1-4(2)3-5/h1H,2H3/b4-1+
C4H4Nr_Olef_2 !! InChI=1S/C4H4N/c1-4(2)3-5/h1-2H2
C4H5N_Olef !! InChI=1S/C4H5N/c1-4(2)3-5/h1H2,2H3
C4H6Nr !! InChI=1S/C4H6N/c1-2-3-4-5/h3H,2H2,1H3
C4H6Nr_1 !! InChI=1S/C4H6N/c1-4(2)3-5/h4H,1H2,2H3/t4-/m0/s1
C4H6Nr_2 !! InChI=1S/C4H6N/c1-4(2)3-5/h4H,1H2,2H3/t4-/m1/s1
C4H6Nr_3 !! InChI=1S/C4H6N/c1-4(2)3-5/h1-2H3
C4H6Nr_Olef!! InChI=1S/C4H6N/c1-3-5-4-2/h1,3-4H,2H3/b3-1+,5-4+
C4H6Nr_Olef_1 !! InChI=1S/C4H6N/c1-3-5-4-2/h1,3-4H,2H3/b3-1+,5-4-
C4H6Nr_Olef_2 !! InChI=1S/C4H6N/c1-3-5-4-2/h1,3-4H,2H3/b3-1-,5-4-
C4H6Nr_Olef_3 !! InChI=1S/C4H6N/c1-3-5-4-2/h1,3-4H,2H3/b3-1-,5-4+
C4H6Nr_Olef_4 !! InChI=1S/C4H6N/c1-3-5-4-2/h3-4H,1-2H2
C4H6Nr_Olef_5 !! InChI=1S/C4H6N/c1-3-5-4-2/h4H,1H2,2H3
C4H6Nr_Olef_6 !! InChI=1S/C4H6N/c1-3-5-4-2/h3H,1H2,2H3
C4H7N_Olef !! InChI=1S/C4H7N/c1-3-5-4-2/h3-4H,1H2,2H3/b5-4+
C4H7N_Olef_1 !! InChI=1S/C4H7N/c1-3-5-4-2/h3-4H,1H2,2H3/b5-4-
C4H7r_Olef !! InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2
C4H7r_Olef_1 !! InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3/b3-1-
C4H7r_Olef_2 !! InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3/b3-1+
C4H7r_Olef_3 !! InChI=1S/C4H7/c1-3-4-2/h1,4H2,2H3
C4H7r_Olef_4 !! InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3
C4H7r_Olef_5 !! InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3/b4-3+
C4H7r_Olef_6 !! InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3/b4-3-
C4H7r_Olef_7 !! InChI=1S/C4H7/c1-4(2)3/h1H,2-3H3
C4H7r_Olef_8 !! InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3
C4H8Nr !! InChI=1S/C4H8N/c1-3-5-4-2/h3-4H,1-2H3
C4H8Nr_1 !! InChI=1S/C4H8N/c1-3-5-4-2/h4H,1,3H2,2H3/b5-4+
C4H8Nr_2 !! InChI=1S/C4H8N/c1-3-5-4-2/h4H,1,3H2,2H3/b5-4-
C4H8Nr_3 !! InChI=1S/C4H8N/c1-3-5-4-2/h3H2,1-2H3
C4H8Nr_Olef!! InChI=1S/C4H8N/c1-3-5-4-2/h3-5H,1H2,2H3
C4H8Nr_Olef_1 !! InChI=1S/C4H8N/c1-3-5-4-2/h3,5H,1-2,4H2
C4H8Nr_Olef_2 !! InChI=1S/C4H8N/c1-3-5-4-2/h1,3,5H,4H2,2H3/b3-1-
C4H8Nr_Olef_3 !! InChI=1S/C4H8N/c1-3-5-4-2/h1,3,5H,4H2,2H3/b3-1+
C4H8Nr_Olef_4 !! InChI=1S/C4H8N/c1-3-5-4-2/h5H,1,4H2,2H3
C4H8Nr_Olef_5 !! InChI=1S/C4H8N/c1-3-5-4-2/h3H,1,4H2,2H3
C4H8_Olef !! InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3
C4H8_Olef_1 !! InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3-
C4H8_Olef_2 !! InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+
C4H8_Olef_3 !! InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3

C4H9N !! InChI=1S/C4H9N/c1-3-5-4-2/h3H,4H2,1-2H3/b5-3+
C4H9N_1 !! InChI=1S/C4H9N/c1-3-5-4-2/h3H,4H2,1-2H3/b5-3-
C4H9N_Olef !! InChI=1S/C4H9N/c1-3-5-4-2/h3,5H,1,4H2,2H3
C4H9r !! InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3
C4H9r_1 !! InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3
C4H9r_2 !! InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3
C4H9r_3 !! InChI=1S/C4H9/c1-4(2)3/h1-3H3
CCNCC !! InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3
CCnjCC !! InChI=1S/C4H10N/c1-3-5-4-2/h3-4H2,1-2H3
CCjNCC !! InChI=1S/C4H10N/c1-3-5-4-2/h3,5H,4H2,1-2H3
CH2CHCN !! InChI=1S/C3H3N/c1-2-3-4/h2H,1H2
CH3CH2CN !! InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3
CH3CHNCH2 !! InChI=1S/C3H6N/c1-3-4-2/h3H,2H2,1H3
CjCNCC !! InChI=1S/C4H10N/c1-3-5-4-2/h5H,1,3-4H2,2H3
CH3CHCN(S) !! InChI=1S/C3H5N/c1-2-3-4/h2-3H,1H3/b3-2-
c-C3H5N !! InChI=1S/C3H5N/c1-3-2-4-3/h2-3H,1H3
HCN !! InChI=1S/CHN/c1-2/h1H
C2H4Nr !! InChI=1S/C2H4N/c1-3-2/h1H,2H3
CH5N !! InChI=1S/CH5N/c1-2/h2H2,1H3
CH4Nr_1 !! InChI=1S/CH4N/c1-2/h2H,1H3
C2H6Nr !! InChI=1S/C2H6N/c1-2-3/h3H,2H2,1H3
H2 !! InChI=1S/H2/h1H
H2O !! InChI=1S/H2O/h1H2
H3N !! InChI=1S/H3N/h1H3
C2H4_Olef !! InChI=1S/C2H4/c1-2/h1-2H2
C2H6Nr_3 !! InChI=1S/C2H6N/c1-2-3/h1-3H2
CHNHr !! InChI=1S/CH2N/c1-2/h1-2H
C2H5r !! InChI=1S/C2H5/c1-2/h1H2,2H3
CH3N !! InChI=1S/CH3N/c1-2/h2H,1H2
C2H4Nr_3 !! InChI=1S/C2H4N/c1-2-3/h3H,1H3
C2H4Nr_1 !! InChI=1S/C2H4N/c1-3-2/h1-2H2
C2H5N_Olef !! InChI=1S/C2H5N/c1-2-3/h2H,1,3H2
H2O2 !! InChI=1S/H2O2/c1-2/h1-2H
Hr !! InChI=1S/H
C2H6 !! InChI=1S/C2H6/c1-2/h1-2H3
H2Nr !! InChI=1S/H2N/h1H2
CH2CHN(S) !! InChI=1S/C2H3N/c1-2-3/h2H,1H2
C2H2Nr !! InChI=1S/C2H2N/c1-2-3/h1H2
CH2Nr !! InChI=1S/CH2N/c1-2/h1H2
C2H6Nr_1 !! InChI=1S/C2H6N/c1-3-2/h3H,1H2,2H3
HOr !! InChI=1S/HO/h1H
Or !! InChI=1S/O
CH3CN !! InChI=1S/C2H3N/c1-2-3/h1H3
HO2r !! InChI=1S/HO2/c1-2/h1H
C2H6Nr_2 !! InChI=1S/C2H6N/c1-2-3/h2H,3H2,1H3
CH3r !! InChI=1S/CH3/h1H3
C2H4Nr_2 !! InChI=1S/C2H4N/c1-2-3/h2-3H,1H2
CH4 !! InChI=1S/CH4/h1H4
C2H5N_2 !! InChI=1S/C2H5N/c1-3-2/h1H2,2H3
c-C2H3N !! InChI=1S/C2H3N/c1-2-3-1/h1H,2H2
C2H3r_Olef !! InChI=1S/C2H3/c1-2/h1H,2H2
C2H4Nr_Olef_2 !! InChI=1S/C2H4N/c1-2-3/h1,3H2
He !! InChI=1S/He
O2 !! InChI=1S/O2/c1-2
CH4Nr !! InChI=1S/CH4N/c1-2/h1-2H2
C2H7N !! InChI=1S/C2H7N/c1-2-3/h2-3H2,1H3
C2H4Nr_4 !! InChI=1S/C2H4N/c1-2-3/h2H,1H3
O3 !! InChI=1S/O3/c1-3-2

CO !! InChI=1S/CO/c1-2
CO2 !! InChI=1S/CO2/c2-1-3
CH2 !! InChI=1S/CH2/h1H2
CH2 (S) !! InChI=1S/CH2/h1H2/S
CH !! InChI=1S/CH/h1H
C !! InChI=1S/C
CH3OH !! InChI=1S/CH4O/c1-2/h2H,1H3
CH3O !! InChI=1S/CH3O/c1-2/h1H3
CH2OH !! InChI=1S/CH3O/c1-2/h2H,1H2
CH2O !! InChI=1S/CH2O/c1-2/h1H2
HCOH !! InChI=1S/CH2O/c1-2/h1-2H
HCO !! InChI=1S/CHO/c1-2/h1H
HOCO !! InChI=1S/CHO2/c2-1-3/h(H,2,3)
HOCHO !! InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)
OCHO !! InChI=1S/CHO2/c2-1-3/h1H
HOCH2O !! InChI=1S/CH3O2/c2-1-3/h2H,1H2
CH3OOH !! InChI=1S/CH4O2/c1-3-2/h2H,1H3
CH3OO !! InChI=1S/CH3O2/c1-3-2/h1H3
CH2OOH !! InChI=1S/CH3O2/c1-3-2/h2H,1H2
C2H2 !! InChI=1S/C2H2/c1-2/h1-2H
H2CC !! InChI=1S/C2H2/c1-2/h1H2
C2H !! InChI=1S/C2H/c1-2/h1H
C2 !! InChI=1S/C2/c1-2
CH3CH2OH !! InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3
CH3CHOH !! InChI=1S/C2H5O/c1-2-3/h2-3H,1H3
CH3CH2O !! InChI=1S/C2H5O/c1-2-3/h2H2,1H3
CH2CH2OH !! InChI=1S/C2H5O/c1-2-3/h3H,1-2H2
CH3CHO !! InChI=1S/C2H4O/c1-2-3/h2H,1H3
CH2CHOH !! InChI=1S/C2H4O/c1-2-3/h2-3H,1H2
cC2H4O !! InChI=1S/C2H4O/c1-2-3-1/h1-2H2
CHCHOH !! InChI=1S/C2H3O/c1-2-3/h1-3H
cC2H3O !! InChI=1S/C2H3O/c1-2-3-1/h1H,2H2
CH2CHO !! InChI=1S/C2H3O/c1-2-3/h2H,1H2
CH3CO !! InChI=1S/C2H3O/c1-2-3/h1H3
CH2CO !! InChI=1S/C2H2O/c1-2-3/h1H2
CHCHO !! InChI=1S/C2H2O/c1-2-3/h1-2H
HCCOH !! InChI=1S/C2H2O/c1-2-3/h1,3H
HCCO !! InChI=1S/C2HO/c1-2-3/h1H
C2O !! InChI=1S/C2O/c1-2-3
CH3CH2OOH !! InChI=1S/C2H6O2/c1-2-4-3/h3H,2H2,1H3
CH3CH2OO !! InChI=1S/C2H5O2/c1-2-4-3/h2H2,1H3
CH3CHOOH !! InChI=1S/C2H5O2/c1-2-4-3/h2-3H,1H3
CH2CH2OOH !! InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2
CH2CHOOH !! InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2
HOCH2CH2OO !! InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2
CH2CHOO !! InChI=1S/C2H3O2/c1-2-4-3/h2H,1H2
OCHCHO !! InChI=1S/C2H2O2/c3-1-2-4/h1-2H
OCHCO !! InChI=1S/C2HO2/c3-1-2-4/h1H
CH3C(O)OOH !! InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3
CH3C(O)OO !! InChI=1S/C2H3O3/c1-2(3)5-4/h1H3
CH3C(O)O !! InChI=1S/C2H3O2/c1-2(3)4/h1H3
NO !! InChI=1S/NO/c1-2
NH !! InChI=1S/HN/h1H
N !! InChI=1S/N
NNH !! InChI=1S/HN2/c1-2/h1H
N2H4 !! InChI=1S/H4N2/c1-2/h1-2H2
N2H3 !! InChI=1S/H3N2/c1-2/h1H,2H2
N2H2 !! InChI=1S/H2N2/c1-2/h1-2H

H2NN !! InChI=1S/H2N2/c1-2/h1H2
NH2OH !! InChI=1S/H3NO/c1-2/h2H,1H2
H2NO !! InChI=1S/H2NO/c1-2/h1H2
HNOH !! InChI=1S/H2NO/c1-2/h1-2H
HNO !! InChI=1S/HNO/c1-2/h1H
HON !! InChI=1S/HNO/c1-2/h2H
NO2 !! InChI=1S/NO2/c2-1-3
HONO !! InChI=1S/H2NO2/c2-1-3/h1-2H
HNO2 !! InChI=1S/HNO2/c2-1-3/h1H
NO3 !! InChI=1S/NO3/c2-1(3)4
HONO2 !! InChI=1S/HNO3/c2-1(3)4/h(H,2,3,4)
N2O !! InChI=1S/N2O/c1-2-3
HNC !! InChI=1S/CHN/c1-2/h2H
CN !! InChI=1S/CN/c1-2
HNCO !! InChI=1S/CHNO/c2-1-3/h2H
HOCN !! InChI=1S/CHNO/c2-1-3/h(H-,2,3)/q-1
HCNO !! InChI=1S/CHNO/c1-2-3/h1H
NCO !! InChI=1S/CNO/c2-1-3
NCN !! InChI=1S/CN2/c2-1-3
HNCN !! InChI=1S/CHN2/c2-1-3/h2H
NCNO !! InChI=1S/CN2O/c2-1-3-4
NCNOH !! InChI=1S/CHN2O/c2-1-3-4/h4H
HNCNH !! InChI=1S/CH2N2/c2-1-3/h2-3H
NCCN !! InChI=1S/C2N2/c3-1-2-4
CH3NO !! InChI=1S/CH3NO/c1-2-3/h1H3
CH2NO !! InChI=1S/CH2NO/c1-2-3/h1H2
C2H5NO !! InChI=1S/C2H5NO/c1-2-3-4/h2H2,1H3
CH3CHNO !! InChI=1S/C2H4NO/c1-2-3-4/h2H,1H3
CH2CHNO !! InChI=1S/C2H3NO/c1-2-3-4/h2H,1H2
CHCHNO !! InChI=1S/C2H2NO/c1-2-3-4/h1-2H
CH3NO2 !! InChI=1S/CH3NO2/c1-2(3)4/h1H3
CH2NO2 !! InChI=1S/CH2NO2/c1-2(3)4/h1H2
C2H5NO2 !! InChI=1S/C2H5NO2/c1-2-3(4)5/h2H2,1H3
CH2CH2NO2 !! InChI=1S/C2H4NO2/c1-2-3(4)5/h1-2H2
CH3CHNO2 !! InChI=1S/C2H4NO2/c1-2-3(4)5/h2H,1H3
CH3ONO !! InChI=1S/CH3NO2/c1-4-2-3/h1H3
CH3ONO2 !! InChI=1S/CH3NO3/c1-5-2(3)4/h1H3
CH3CH2ONO !! InChI=1S/C2H5NO2/c1-2-5-3-4/h2H2,1H3
CH3CH2ONO2 !! InChI=1S/C2H5NO3/c1-2-6-3(4)5/h2H2,1H3
CH3CHNH !! InChI=1S/C2H5N/c1-2-3/h2-3H,1H3
CHCHNH2 !! InChI=1S/C2H4N/c1-2-3/h1-2H,3H2
CHCNH2 !! InChI=1S/C2H3N/c1-2-3/h1H,3H2
CH2CNH !! InChI=1S/C2H3N/c1-2-3/h3H,1H2
CH2CHN(S)_m0 !! InChI=1S/C2H3N/c1-2-3/h2H,1H2/S
CHCNH !! InChI=1S/C2H2N/c1-2-3/h1,3H
H2NCHO !! InChI=1S/CH3NO/c2-1-3/h1H,(H2,2,3)
H2NCO !! InChI=1S/CH2NO/c2-1-3/h(H2,2,3)
CH3NHCH3 !! InChI=1S/C2H7N/c1-3-2/h3H,1-2H3
CH3NCH3 !! InChI=1S/C2H6N/c1-3-2/h1-2H3
AR !! InChI=1S/Ar
N2 !! InChI=1S/N2/c1-2
COOjCNCC !! InChI=1S/C4H10NO2/c1-2-5-3-4-7-6/h5H,2-4H2,1H3
CCOOjNCC !! InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h4-5H,3H2,1-2H3/t4-
/m1/s1
CCNOOjCC !! InChI=1S/C4H10NO2/c1-3-5(4-2)7-6/h3-4H2,1-2H3
CCOONjC !! InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h3-6H,1-2H3/t4-/m1/s1
CCdONCC !! InChI=1S/C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,(H,5,6)
OOCdNCC !! InChI=1S/C3H7NO2/c1-2-4-3-6-5/h3,5H,2H2,1H3/b4-3-

CCOONjCC !! InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h4,6H,3H2,1-2H3
OdCdNCC !! InChI=1S/C3H5NO/c1-2-4-3-5/h2H2,1H3
OjCdNCC !! InChI=1S/C3H6NO/c1-2-4-3-5/h3H,2H2,1H3
CCdONjCC !! InChI=1S/C4H8NO/c1-3-5-4(2)6/h3H2,1-2H3

END

THERMO ALL
298.0 600.0 1000.0

C3H8 H 8 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
2.60098976E-01 3.22734441E-02-1.17435416E-05-1.41738797E-09 1.40645746E-
12 2
-1.40333725E+04 2.20015879E+01 2.60098976E-01 3.22734441E-02-1.17435416E-
05 3
-1.41738797E-09 1.40645746E-12-1.40333725E+04 2.20015879E+01
4

C2H4Nr_Olef H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
6.92724781E-01 3.01699310E-02-2.85923239E-05 1.47299485E-08-3.08274915E-
12 2
3.65509416E+04 2.12208611E+01 6.92724781E-01 3.01699310E-02-2.85923239E-
05 3
1.47299485E-08-3.08274915E-12 3.65509416E+04 2.12208611E+01
4

C2H4Nr_Olef_1 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
6.92724781E-01 3.01699310E-02-2.85923239E-05 1.47299485E-08-3.08274915E-
12 2
3.65509416E+04 2.12208611E+01 6.92724781E-01 3.01699310E-02-2.85923239E-
05 3
1.47299485E-08-3.08274915E-12 3.65509416E+04 2.12208611E+01
4

C2H5N H 5 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.77260119E+00 1.81704408E-02 4.95289956E-08-7.61920975E-09 2.84106378E-
12 2
3.62311833E+03 1.62292539E+01 1.77260119E+00 1.81704408E-02 4.95289956E-
08 3
-7.61920975E-09 2.84106378E-12 3.62311833E+03 1.62292539E+01
4

C2H5N_1 H 5 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.77260119E+00 1.81704408E-02 4.95289956E-08-7.61920975E-09 2.84106378E-
12 2
3.62311833E+03 1.62292539E+01 1.77260119E+00 1.81704408E-02 4.95289956E-
08 3
-7.61920975E-09 2.84106378E-12 3.62311833E+03 1.62292539E+01
4

C3H2Nr_Olef H 2 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.43090688E+00 1.64982178E-02-9.57159317E-06 2.08789332E-09 6.14322410E-
14 2
4.94770970E+04 9.66812249E+00 3.43090688E+00 1.64982178E-02-9.57159317E-
06 3
2.08789332E-09 6.14322410E-14 4.94770970E+04 9.66812249E+00
4

C3H2Nr_Olef_1 H 2 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.61116654E+00 1.25936035E-02-8.72172140E-06 3.25193397E-09-5.08193444E-
13 2
5.19993385E+04 2.09066926E+01 1.61116654E+00 1.25936035E-02-8.72172140E-
06 3
3.25193397E-09-5.08193444E-13 5.19993385E+04 2.09066926E+01
4

C3H2Nr_Olef_2 H 2 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.61116654E+00 1.25936035E-02-8.72172140E-06 3.25193397E-09-5.08193444E-
13 2
5.19993385E+04 2.09066926E+01 1.61116654E+00 1.25936035E-02-8.72172140E-
06 3
3.25193397E-09-5.08193444E-13 5.19993385E+04 2.09066926E+01
4

C3H4Nr H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
7.35564706E-02 1.15371456E-02-1.03660754E-05 5.46754962E-09-1.20930314E-
12 2
3.15394481E+04 3.33542057E+01 7.35564706E-02 1.15371456E-02-1.03660754E-
05 3
5.46754962E-09-1.20930314E-12 3.15394481E+04 3.33542057E+01
4

C3H4Nr_1 H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.92234636E+00 2.49600727E-02-1.39360320E-05 3.10599975E-09-3.26982276E-
14 2
2.54512332E+04 1.75856533E+01 1.92234636E+00 2.49600727E-02-1.39360320E-
05 3
3.10599975E-09-3.26982276E-14 2.54512332E+04 1.75856533E+01
4

C3H4Nr_Olef H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.46650277E+00 2.32167064E-02-1.57870865E-05 5.82718087E-09-9.06691230E-
13 2
4.94993778E+04 2.95130756E+01 1.46650277E+00 2.32167064E-02-1.57870865E-
05 3

5.82718087E-09-9.06691230E-13 4.94993778E+04 2.95130756E+01
4

C3H4Nr_Olef_1 H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.46650277E+00 2.32167064E-02-1.57870865E-05 5.82718087E-09-9.06691230E-
13 2
4.94993778E+04 2.95130756E+01 1.46650277E+00 2.32167064E-02-1.57870865E-
05 3
5.82718087E-09-9.06691230E-13 4.94993778E+04 2.95130756E+01
4

C3H4Nr_Olef_2 H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
9.58417608E-01 1.35222050E-02-2.88267291E-06-3.10176961E-09 1.42842302E-
12 2
4.37538168E+04 2.97103089E+01 9.58417608E-01 1.35222050E-02-2.88267291E-
06 3
-3.10176961E-09 1.42842302E-12 4.37538168E+04 2.97103089E+01
4

C3H4Nr_Olef_3 H 4 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-7.02179035E-02 1.01353614E-02-5.99780377E-06 1.63439978E-09-1.16650805E-
13 2
4.05973800E+04 2.71823328E+01-7.02179035E-02 1.01353614E-02-5.99780377E-
06 3
1.63439978E-09-1.16650805E-13 4.05973800E+04 2.71823328E+01
4

C3H5N_Olef H 5 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-7.86149096E-01 4.68948295E-02-4.93477507E-05 2.81475996E-08-6.43650131E-
12 2
1.83798018E+04 2.71244980E+01-7.86149096E-01 4.68948295E-02-4.93477507E-
05 3
2.81475996E-08-6.43650131E-12 1.83798018E+04 2.71244980E+01
4

C3H5r_Olef H 5 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
-1.19903396E+00 3.79491187E-02-3.48340701E-05 1.79227691E-08-3.83200861E-
12 2
1.91277180E+04 2.79365329E+01-1.19903396E+00 3.79491187E-02-3.48340701E-
05 3
1.79227691E-08-3.83200861E-12 1.91277180E+04 2.79365329E+01
4

C3H5r_Olef_1 H 5 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
1.99636488E+00 2.07677811E-02-6.74136366E-06-1.60484032E-09 1.07006168E-
12 2

2.89258435E+04 1.56676088E+01 1.99636488E+00 2.07677811E-02-6.74136366E-
06 3
-1.60484032E-09 1.07006168E-12 2.89258435E+04 1.56676088E+01
4

C3H5r_Olef_2 H 5 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
1.30344198E+00 2.53783482E-02-1.51740091E-05 4.56103524E-09-5.19532458E-
13 2
3.07465682E+04 1.82758199E+01 1.30344198E+00 2.53783482E-02-1.51740091E-
05 3
4.56103524E-09-5.19532458E-13 3.07465682E+04 1.82758199E+01
4

C3H5r_Olef_3 H 5 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
1.30344198E+00 2.53783482E-02-1.51740091E-05 4.56103524E-09-5.19532458E-
13 2
3.07465682E+04 1.82758199E+01 1.30344198E+00 2.53783482E-02-1.51740091E-
05 3
4.56103524E-09-5.19532458E-13 3.07465682E+04 1.82758199E+01
4

C3H6Nr H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.72015440E-02 1.08557280E-02-3.12303052E-06-1.15158387E-09 6.47109287E-
13 2
2.50070881E+04 2.98226022E+01 4.72015440E-02 1.08557280E-02-3.12303052E-
06 3
-1.15158387E-09 6.47109287E-13 2.50070881E+04 2.98226022E+01
4

C3H6Nr_1 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-3.48003068E-01 3.73420701E-02-2.23537534E-05 5.42968658E-09-1.16978394E-
13 2
2.35513808E+04 2.76575160E+01-3.48003068E-01 3.73420701E-02-2.23537534E-
05 3
5.42968658E-09-1.16978394E-13 2.35513808E+04 2.76575160E+01
4

C3H6Nr_2 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.36207527E-01 2.15686789E-02-6.08796145E-06-2.37910249E-09 1.30958019E-
12 2
2.91636308E+04 2.76312068E+01 1.36207527E-01 2.15686789E-02-6.08796145E-
06 3
-2.37910249E-09 1.30958019E-12 2.91636308E+04 2.76312068E+01
4

C3H6Nr_3 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1

-7.11073041E-02 2.21602485E-02-1.74314405E-05 8.04279652E-09-1.60780093E-
12 2
3.06751895E+04 3.32408532E+01-7.11073041E-02 2.21602485E-02-1.74314405E-
05 3
8.04279652E-09-1.60780093E-12 3.06751895E+04 3.32408532E+01
4

C3H6Nr_4 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.72015440E-02 1.08557280E-02-3.12303052E-06-1.15158387E-09 6.47109287E-
13 2
2.95894599E+04 2.91370508E+01 4.72015440E-02 1.08557280E-02-3.12303052E-
06 3
-1.15158387E-09 6.47109287E-13 2.95894599E+04 2.91370508E+01
4

C3H6Nr_Olef H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
3.63747867E+04 2.16426925E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 3.63747867E+04 2.16426925E+01
4

C3H6Nr_Olef_1 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
3.63747867E+04 2.16426925E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 3.63747867E+04 2.16426925E+01
4

C3H6Nr_Olef_2 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
9.58417608E-01 1.35222050E-02-2.88267291E-06-3.10176961E-09 1.42842302E-
12 2
2.75050401E+04 2.75738951E+01 9.58417608E-01 1.35222050E-02-2.88267291E-
06 3
-3.10176961E-09 1.42842302E-12 2.75050401E+04 2.75738951E+01
4

C3H6Nr_Olef_3 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.75272834E+00 2.83279569E-02-1.01415842E-05-2.22097224E-09 1.69792490E-
12 2
3.31592132E+04 2.10953615E+01 1.75272834E+00 2.83279569E-02-1.01415842E-
05 3
-2.22097224E-09 1.69792490E-12 3.31592132E+04 2.10953615E+01
4

C3H6_Olef H 6 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
7.84532100E-01 2.58009276E-02-8.82001727E-06-1.94848605E-09 1.41298272E-
12 2
1.10702154E+03 2.02642658E+01 7.84532100E-01 2.58009276E-02-8.82001727E-
06 3
-1.94848605E-09 1.41298272E-12 1.10702154E+03 2.02642658E+01
4

C3H7N H 7 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.08745017E+00 2.69707243E-02 6.30766249E-07-1.20717350E-08 4.46591953E-
12 2
4.44318632E+03 2.21977922E+01 1.08745017E+00 2.69707243E-02 6.30766249E-
07 3
-1.20717350E-08 4.46591953E-12 4.44318632E+03 2.21977922E+01
4

C3H7N_1 H 7 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.91003209E+00 2.30021614E-02 4.18521489E-06-1.33931701E-08 4.60862359E-
12 2
2.22773439E+03 1.22696382E+01 2.91003209E+00 2.30021614E-02 4.18521489E-
06 3
-1.33931701E-08 4.60862359E-12 2.22773439E+03 1.22696382E+01
4

C3H7N_2 H 7 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.16060582E+00 3.51307211E-02-1.79033192E-05 2.84458081E-09 3.82178219E-
13 2
4.38149178E+03 2.08509742E+01 1.16060582E+00 3.51307211E-02-1.79033192E-
05 3
2.84458081E-09 3.82178219E-13 4.38149178E+03 2.08509742E+01
4

C3H7N_Olef H 7 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
6.55264413E-01 3.69640093E-02-2.00896010E-05 4.03866489E-09 1.51966115E-
13 2
5.35653359E+03 2.20173930E+01 6.55264413E-01 3.69640093E-02-2.00896010E-
05 3
4.03866489E-09 1.51966115E-13 5.35653359E+03 2.20173930E+01
4

C3H7r H 7 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
5.80860940E-01 3.19920146E-02-1.77417344E-05 4.49242291E-09-3.01287613E-
13 2
1.06776220E+04 2.28329463E+01 5.80860940E-01 3.19920146E-02-1.77417344E-
05 3
4.49242291E-09-3.01287613E-13 1.06776220E+04 2.28329463E+01
4

C3H7r_1 H 7 C 3 G 3.0E+02 1.5E+03 1.5E+03
1
1.53093280E+00 2.24047386E-02 1.61734693E-06 -1.04904377E-08 3.71726490E-
12 2
9.22178050E+03 1.93615601E+01 1.53093280E+00 2.24047386E-02 1.61734693E-
06 3
-1.04904377E-08 3.71726490E-12 9.22178050E+03 1.93615601E+01
4

C3H8Nr H 8 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.15305307E-01 2.16400675E-02 -6.16701125E-06 -2.34113512E-09 1.30189938E-
12 2
1.39288270E+04 3.37458162E+01 1.15305307E-01 2.16400675E-02 -6.16701125E-
06 3
-2.34113512E-09 1.30189938E-12 1.39288270E+04 3.37458162E+01
4

C3H8Nr_1 H 8 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.22757132E+00 3.23896117E-02 -1.23873785E-05 -1.18311521E-09 1.42854772E-
12 2
1.78474451E+04 1.09856308E+01 3.22757132E+00 3.23896117E-02 -1.23873785E-
05 3
-1.18311521E-09 1.42854772E-12 1.78474451E+04 1.09856308E+01
4

C3H8Nr_2 H 8 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.20276627E+00 3.73672244E-02 -2.15064820E-05 5.83535262E-09 -4.74444801E-
13 2
1.34686654E+04 1.55371191E+01 2.20276627E+00 3.73672244E-02 -2.15064820E-
05 3
5.83535262E-09 -4.74444801E-13 1.34686654E+04 1.55371191E+01
4

C4H4Nr_Olef H 4 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-4.65888743E-01 3.50073445E-02 -3.28816952E-05 1.63411782E-08 -3.28484691E-
12 2
4.72173062E+04 3.02725663E+01 -4.65888743E-01 3.50073445E-02 -3.28816952E-
05 3
1.63411782E-08 -3.28484691E-12 4.72173062E+04 3.02725663E+01
4

C4H4Nr_Olef_1 H 4 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-4.65888743E-01 3.50073445E-02 -3.28816952E-05 1.63411782E-08 -3.28484691E-
12 2
4.72173062E+04 3.02725663E+01 -4.65888743E-01 3.50073445E-02 -3.28816952E-
05 3

1.63411782E-08-3.28484691E-12 4.72173062E+04 3.02725663E+01
4

C4H4Nr_Olef_2 H 4 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-3.26052701E+00 4.71408686E-02-5.00141678E-05 2.70136574E-08-5.74343438E-
12 2
3.55191610E+04 4.18701366E+01-3.26052701E+00 4.71408686E-02-5.00141678E-
05 3
2.70136574E-08-5.74343438E-12 3.55191610E+04 4.18701366E+01
4

C4H5N_Olef H 5 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-1.11863768E+00 3.59359461E-02-2.70426468E-05 9.98747460E-09-1.34823044E-
12 2
1.71784587E+04 3.28340542E+01-1.11863768E+00 3.59359461E-02-2.70426468E-
05 3
9.98747460E-09-1.34823044E-12 1.71784587E+04 3.28340542E+01
4

C4H6Nr H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.06927367E+00 1.75438586E-02-2.11270373E-06-5.04995022E-09 2.03200717E-
12 2
2.37782511E+04 2.89921364E+01 1.06927367E+00 1.75438586E-02-2.11270373E-
06 3
-5.04995022E-09 2.03200717E-12 2.37782511E+04 2.89921364E+01
4

C4H6Nr_1 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.20758015E-01 2.23928737E-02-1.34891060E-05 4.31596575E-09-5.62193858E-
13 2
2.78616127E+04 3.29403726E+01 1.20758015E-01 2.23928737E-02-1.34891060E-
05 3
4.31596575E-09-5.62193858E-13 2.78616127E+04 3.29403726E+01
4

C4H6Nr_2 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.20758015E-01 2.23928737E-02-1.34891060E-05 4.31596575E-09-5.62193858E-
13 2
2.78616127E+04 3.29403726E+01 1.20758015E-01 2.23928737E-02-1.34891060E-
05 3
4.31596575E-09-5.62193858E-13 2.78616127E+04 3.29403726E+01
4

C4H6Nr_3 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.68651215E+00 2.90881437E-02-6.97705110E-06-5.45217423E-09 2.59301954E-
12 2

2.00777422E+04 1.56576996E+01 2.68651215E+00 2.90881437E-02-6.97705110E-
06 3
-5.45217423E-09 2.59301954E-12 2.00777422E+04 1.56576996E+01
4

C4H6Nr_Olef H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
4.49141139E+04 2.72834595E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 4.49141139E+04 2.72834595E+01
4

C4H6Nr_Olef_1 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
4.49141139E+04 2.72834595E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 4.49141139E+04 2.72834595E+01
4

C4H6Nr_Olef_2 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
4.49141139E+04 2.72834595E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 4.49141139E+04 2.72834595E+01
4

C4H6Nr_Olef_3 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.67927031E+00 2.33779429E-02-1.17657021E-05 2.06238273E-09 1.46596652E-
13 2
4.49141139E+04 2.72834595E+01 1.67927031E+00 2.33779429E-02-1.17657021E-
05 3
2.06238273E-09 1.46596652E-13 4.49141139E+04 2.72834595E+01
4

C4H6Nr_Olef_4 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-2.53987567E+00 5.37371331E-02-2.93885749E-05-3.69432855E-10 3.24940755E-
12 2
2.94358183E+04 3.57278210E+01-2.53987567E+00 5.37371331E-02-2.93885749E-
05 3
-3.69432855E-10 3.24940755E-12 2.94358183E+04 3.57278210E+01
4

C4H6Nr_Olef_5 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1

-2.30163596E-02 2.09910894E-02-9.12083429E-06 4.82815911E-10 5.30458482E-13 2
3.89882269E+04 3.22725356E+01-2.30163596E-02 2.09910894E-02-9.12083429E-06 3
4.82815911E-10 5.30458482E-13 3.89882269E+04 3.22725356E+01
4

C4H6Nr_Olef_6 H 6 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.02652137E+00 2.43065445E-02-5.92665364E-06-4.29132085E-09 2.08321312E-12 2
3.92544444E+04 3.11078058E+01 1.02652137E+00 2.43065445E-02-5.92665364E-06 3
-4.29132085E-09 2.08321312E-12 3.92544444E+04 3.11078058E+01
4

C4H7N_Olef H 7 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.27043812E+00 3.32067665E-02-7.83213122E-06-6.93701858E-09 3.30568213E-12 2
1.39588534E+04 1.80519449E+01 2.27043812E+00 3.32067665E-02-7.83213122E-06 3
-6.93701858E-09 3.30568213E-12 1.39588534E+04 1.80519449E+01
4

C4H7N_Olef_1 H 7 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.02652137E+00 2.43065445E-02-5.92665364E-06-4.29132085E-09 2.08321312E-12 2
1.48752663E+04 2.98449474E+01 1.02652137E+00 2.43065445E-02-5.92665364E-06 3
-4.29132085E-09 2.08321312E-12 1.48752663E+04 2.98449474E+01
4

C4H7r_Olef H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
6.85675508E-01 3.82337288E-02-2.35791631E-05 6.94401806E-09-6.64944634E-13 2
2.35377714E+04 2.41620920E+01 6.85675508E-01 3.82337288E-02-2.35791631E-05 3
6.94401806E-09-6.64944634E-13 2.35377714E+04 2.41620920E+01
4

C4H7r_Olef_1 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
2.23838294E-01 4.12233936E-02-2.93782439E-05 1.16296033E-08-1.99167161E-12 2
2.81314826E+04 2.51107898E+01 2.23838294E-01 4.12233936E-02-2.93782439E-05 3
1.16296033E-08-1.99167161E-12 2.81314826E+04 2.51107898E+01
4

C4H7r_Olef_2 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
2.23838294E-01 4.12233936E-02-2.93782439E-05 1.16296033E-08-1.99167161E-
12 2
2.81314826E+04 2.51107898E+01 2.23838294E-01 4.12233936E-02-2.93782439E-
05 3
1.16296033E-08-1.99167161E-12 2.81314826E+04 2.51107898E+01
4

C4H7r_Olef_3 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
9.57852542E-01 3.60785892E-02-1.97614583E-05 4.42199739E-09-8.84416457E-
14 2
2.62896407E+04 2.23956971E+01 9.57852542E-01 3.60785892E-02-1.97614583E-
05 3
4.42199739E-09-8.84416457E-14 2.62896407E+04 2.23956971E+01
4

C4H7r_Olef_4 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
8.81392301E-02 3.94443726E-02-2.30426165E-05 5.68619092E-09-2.20009144E-
13 2
1.47113675E+04 2.49428465E+01 8.81392301E-02 3.94443726E-02-2.30426165E-
05 3
5.68619092E-09-2.20009144E-13 1.47113675E+04 2.49428465E+01
4

C4H7r_Olef_5 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
3.36335658E+00 2.27463811E-02 3.53536840E-06-1.25205232E-08 4.31331324E-
12 2
2.49442373E+04 1.15902548E+01 3.36335658E+00 2.27463811E-02 3.53536840E-
06 3
-1.25205232E-08 4.31331324E-12 2.49442373E+04 1.15902548E+01
4

C4H7r_Olef_6 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
3.36335658E+00 2.27463811E-02 3.53536840E-06-1.25205232E-08 4.31331324E-
12 2
2.49442373E+04 1.15902548E+01 3.36335658E+00 2.27463811E-02 3.53536840E-
06 3
-1.25205232E-08 4.31331324E-12 2.49442373E+04 1.15902548E+01
4

C4H7r_Olef_7 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
1.70716253E+00 3.47581506E-02-1.97859452E-05 5.43546920E-09-5.17114561E-
13 2
2.63759683E+04 1.75511134E+01 1.70716253E+00 3.47581506E-02-1.97859452E-
05 3
5.43546920E-09-5.17114561E-13 2.63759683E+04 1.75511134E+01
4

C4H7r_Olef_8 H 7 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
-1.89463308E+00 5.04738314E-02-4.33062176E-05 2.10372789E-08-4.32675385E-
12 2
1.50952180E+04 3.29066797E+01-1.89463308E+00 5.04738314E-02-4.33062176E-
05 3
2.10372789E-08-4.32675385E-12 1.50952180E+04 3.29066797E+01
4

C4H8Nr H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.15305307E-01 2.16400675E-02-6.16701125E-06-2.34113512E-09 1.30189938E-
12 2
2.14458403E+04 3.16891612E+01 1.15305307E-01 2.16400675E-02-6.16701125E-
06 3
-2.34113512E-09 1.30189938E-12 2.14458403E+04 3.16891612E+01
4

C4H8Nr_1 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.41660234E-01 2.23214851E-02-1.34100562E-05 4.27799837E-09-5.54513048E-
13 2
2.60899256E+04 3.10112371E+01 1.41660234E-01 2.23214851E-02-1.34100562E-
05 3
4.27799837E-09-5.54513048E-13 2.60899256E+04 3.10112371E+01
4

C4H8Nr_2 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.41660234E-01 2.23214851E-02-1.34100562E-05 4.27799837E-09-5.54513048E-
13 2
2.60899256E+04 3.10112371E+01 1.41660234E-01 2.23214851E-02-1.34100562E-
05 3
4.27799837E-09-5.54513048E-13 2.60899256E+04 3.10112371E+01
4

C4H8Nr_3 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.15305307E-01 2.16400675E-02-6.16701125E-06-2.34113512E-09 1.30189938E-
12 2
2.50900875E+04 3.05345477E+01 1.15305307E-01 2.16400675E-02-6.16701125E-
06 3
-2.34113512E-09 1.30189938E-12 2.50900875E+04 3.05345477E+01
4

C4H8Nr_Olef H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.00561915E+00 2.43779331E-02-6.00570344E-06-4.25335348E-09 2.07553231E-
12 2
2.29973267E+04 2.95249932E+01 1.00561915E+00 2.43779331E-02-6.00570344E-
06 3

-4.25335348E-09 2.07553231E-12 2.29973267E+04 2.95249932E+01
4

C4H8Nr_Olef_1 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.03197408E+00 2.50593507E-02-1.32487484E-05 2.36578001E-09 2.19119879E-
13 2
2.85554812E+04 2.84982797E+01 1.03197408E+00 2.50593507E-02-1.32487484E-
05 3
2.36578001E-09 2.19119879E-13 2.85554812E+04 2.84982797E+01
4

C4H8Nr_Olef_2 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.65836809E+00 2.34493315E-02-1.18447519E-05 2.10035010E-09 1.38915842E-
13 2
3.32153126E+04 2.41972440E+01 1.65836809E+00 2.34493315E-02-1.18447519E-
05 3
2.10035010E-09 1.38915842E-13 3.32153126E+04 2.41972440E+01
4

C4H8Nr_Olef_3 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.65836809E+00 2.34493315E-02-1.18447519E-05 2.10035010E-09 1.38915842E-
13 2
3.32153126E+04 2.41972440E+01 1.65836809E+00 2.34493315E-02-1.18447519E-
05 3
2.10035010E-09 1.38915842E-13 3.32153126E+04 2.41972440E+01
4

C4H8Nr_Olef_4 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-2.30163596E-02 2.09910894E-02-9.12083429E-06 4.82815911E-10 5.30458482E-
13 2
3.10983681E+04 3.45697351E+01-2.30163596E-02 2.09910894E-02-9.12083429E-
06 3
4.82815911E-10 5.30458482E-13 3.10983681E+04 3.45697351E+01
4

C4H8Nr_Olef_5 H 8 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.72015440E-02 1.08557280E-02-3.12303052E-06-1.15158387E-09 6.47109287E-
13 2
2.15673028E+04 3.01878506E+01 4.72015440E-02 1.08557280E-02-3.12303052E-
06 3
-1.15158387E-09 6.47109287E-13 2.15673028E+04 3.01878506E+01
4

C4H8_Olef H 8 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
-1.08006966E-01 4.13532430E-02-2.32027113E-05 5.58267411E-09-2.38444872E-
13 2

-1.62222653E+03 2.60888575E+01-1.08006966E-01 4.13532430E-02-2.32027113E-05 3
5.58267411E-09-2.38444872E-13-1.62222653E+03 2.60888575E+01
4

C4H8_Olef_1 H 8 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
1.46562297E+00 2.91114952E-02 1.77855555E-07-1.21518272E-08 4.48104297E-12 2
-2.58706875E+03 1.88825108E+01 1.46562297E+00 2.91114952E-02 1.77855555E-07 3
-1.21518272E-08 4.48104297E-12-2.58706875E+03 1.88825108E+01
4

C4H8_Olef_2 H 8 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
1.86884826E+00 3.08032309E-02-5.27659723E-06-7.15031517E-09 3.00899207E-12 2
-3.22448919E+03 1.60415884E+01 1.86884826E+00 3.08032309E-02-5.27659723E-06 3
-7.15031517E-09 3.00899207E-12-3.22448919E+03 1.60415884E+01
4

C4H8_Olef_3 H 8 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
7.39777888E-01 3.80148356E-02-1.87260932E-05 2.96605872E-09 3.33289105E-13 2
-3.81788859E+03 2.05495183E+01 7.39777888E-01 3.80148356E-02-1.87260932E-05 3
2.96605872E-09 3.33289105E-13-3.81788859E+03 2.05495183E+01
4

C4H9N H 9 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.15305307E-01 2.16400675E-02-6.16701125E-06-2.34113512E-09 1.30189938E-12 2
7.10909467E+02 2.92716893E+01 1.15305307E-01 2.16400675E-02-6.16701125E-06 3
-2.34113512E-09 1.30189938E-12 7.10909467E+02 2.92716893E+01
4

C4H9N_1 H 9 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.08973599E+00 4.44188721E-02-2.02879256E-05 1.19452209E-09 1.19762893E-12 2
-2.76083047E+03 2.16341436E+01 1.08973599E+00 4.44188721E-02-2.02879256E-05 3
1.19452209E-09 1.19762893E-12-2.76083047E+03 2.16341436E+01
4

C4H9N_Olef H 9 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1

1.00561915E+00 2.43779331E-02-6.00570344E-06-4.25335348E-09 2.07553231E-
12 2
3.17646508E+03 2.67587319E+01 1.00561915E+00 2.43779331E-02-6.00570344E-
06 3
-4.25335348E-09 2.07553231E-12 3.17646508E+03 2.67587319E+01
4

C4H9r H 9 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
-1.61347925E-01 4.58555388E-02-2.75064719E-05 7.71362131E-09-6.49272537E-
13 2
7.65705668E+03 2.81828671E+01-1.61347925E-01 4.58555388E-02-2.75064719E-
05 3
7.71362131E-09-6.49272537E-13 7.65705668E+03 2.81828671E+01
4

C4H9r_1 H 9 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
1.04243864E+00 3.60961945E-02-9.58208915E-06-5.33541906E-09 2.70432271E-
12 2
6.76782011E+03 2.40147460E+01 1.04243864E+00 3.60961945E-02-9.58208915E-
06 3
-5.33541906E-09 2.70432271E-12 6.76782011E+03 2.40147460E+01
4

C4H9r_2 H 9 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
-3.00055241E-01 4.88856380E-02-3.46000000E-05 1.36216516E-08-2.30569890E-
12 2
7.13446417E+03 2.70854087E+01-3.00055241E-01 4.88856380E-02-3.46000000E-
05 3
1.36216516E-08-2.30569890E-12 7.13446417E+03 2.70854087E+01
4

C4H9r_3 H 9 C 4 G 3.0E+02 1.5E+03 1.5E+03
1
2.97739732E+00 2.38823967E-02 1.26659517E-05-2.17373736E-08 6.97814703E-
12 2
4.35458440E+03 1.12569824E+01 2.97739732E+00 2.38823967E-02 1.26659517E-
05 3
-2.17373736E-08 6.97814703E-12 4.35458440E+03 1.12569824E+01
4

CCNCC H 11 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.24289107E+00 4.24844977E-02-1.12249484E-05-6.35773265E-09 3.23111096E-
12 2
-1.09387793E+04 1.10425127E+01 3.24289107E+00 4.24844977E-02-1.12249484E-
05 3
-6.35773265E-09 3.23111096E-12-1.09387793E+04 1.10425127E+01
4

CCNjCC H 10 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.45008801E+00 4.21322978E-02-1.35848326E-05-4.27888143E-09 2.68793717E-
12 2
1.00296224E+04 1.68425278E+01 2.45008801E+00 4.21322978E-02-1.35848326E-
05 3
-4.27888143E-09 2.68793717E-12 1.00296224E+04 1.68425278E+01
4

CCjNCC H 10 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
6.03298722E+00 3.04072375E-02 3.02095319E-06-1.53079362E-08 5.43925528E-
12 2
8.19639311E+03 1.98634422E+00 6.03298722E+00 3.04072375E-02 3.02095319E-
06 3
-1.53079362E-08 5.43925528E-12 8.19639311E+03 1.98634422E+00
4

CH2CHCN H 3 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.05999175E+00 2.78475862E-02-2.29695218E-05 1.05087769E-08-2.03236644E-
12 2
2.14425210E+04 1.94028065E+01 1.05999175E+00 2.78475862E-02-2.29695218E-
05 3
1.05087769E-08-2.03236644E-12 2.14425210E+04 1.94028065E+01
4

CH3CH2CN H 5 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.35782830E+00 2.95260499E-02-1.75880304E-05 5.04776957E-09-4.90992831E-
13 2
5.29611891E+03 1.85093934E+01 1.35782830E+00 2.95260499E-02-1.75880304E-
05 3
5.04776957E-09-4.90992831E-13 5.29611891E+03 1.85093934E+01
4

CH3CHNCH2 H 6 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.15711425E+00 3.22906353E-02-1.52100899E-05 8.69606992E-10 9.63446126E-
13 2
2.10487825E+04 2.05470884E+01 1.15711425E+00 3.22906353E-02-1.52100899E-
05 3
8.69606992E-10 9.63446126E-13 2.10487825E+04 2.05470884E+01
4

CjCNCC H 10 C 4 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.45161170E+00 3.97417488E-02-1.40073857E-05-2.51093119E-09 2.03284517E-
12 2
1.44156991E+04 6.63879123E+00 4.45161170E+00 3.97417488E-02-1.40073857E-
05 3
-2.51093119E-09 2.03284517E-12 1.44156991E+04 6.63879123E+00
4

CH3CHCN(S) H 5 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.31308102E+00 3.10442228E-02-1.68281716E-05 2.68394434E-09 4.47563917E-
13 2
3.26748575E+04 1.81997492E+01 1.31308102E+00 3.10442228E-02-1.68281716E-
05 3
2.68394434E-09 4.47563917E-13 3.26748575E+04 1.81997492E+01
4

c-C3H5N H 5 C 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.01058459E-01 3.31703891E-02-1.88291725E-05 3.69449940E-09 2.38894701E-
13 2
2.77808738E+04 2.29663161E+01 1.01058459E-01 3.31703891E-02-1.88291725E-
05 3
3.69449940E-09 2.38894701E-13 2.77808738E+04 2.29663161E+01
4

HCN H 1 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.24486580E+00 9.14786121E-03-1.06463659E-05 6.99978269E-09-1.79489038E-
12 2
1.52233093E+04 9.08117134E+00 2.24486580E+00 9.14786121E-03-1.06463659E-
05 3
6.99978269E-09-1.79489038E-12 1.52233093E+04 9.08117134E+00
4

C2H4Nr H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.73844387E+00 1.46191950E-02-6.39423274E-07-5.14981309E-09 1.92480626E-
12 2
3.32410303E+04 1.18894555E+01 2.73844387E+00 1.46191950E-02-6.39423274E-
07 3
-5.14981309E-09 1.92480626E-12 3.32410303E+04 1.18894555E+01
4

CH5N H 5 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.19204799E+00 1.20842195E-02 3.60439929E-06-7.92224326E-09 2.61342724E-
12 2
-3.54666142E+03 1.28610299E+01 2.19204799E+00 1.20842195E-02 3.60439929E-
06 3
-7.92224326E-09 2.61342724E-12-3.54666142E+03 1.28610299E+01
4

CH4Nr_1 H 4 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.62722498E+00 8.20764804E-03 6.69086954E-06-9.65858634E-09 3.03875845E-
12 2
2.09293039E+04 1.19207837E+01 2.62722498E+00 8.20764804E-03 6.69086954E-
06 3

-9.65858634E-09 3.03875845E-12 2.09293039E+04 1.19207837E+01
4

C2H6Nr H 6 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.91345310E+00 2.28163329E-02-5.94922878E-06-3.51407973E-09 1.77989547E-
12 2
1.68461662E+04 1.70841293E+01 1.91345310E+00 2.28163329E-02-5.94922878E-
06 3
-3.51407973E-09 1.77989547E-12 1.68461662E+04 1.70841293E+01
4

H2 H 2 G 3.0E+02 1.5E+03 1.5E+03
1
3.46563485E+00 2.98571180E-04-8.75520407E-07 9.64903160E-10-2.81201547E-
13 2
-1.04006338E+03-4.13063173E+00 3.46563485E+00 2.98571180E-04-8.75520407E-
07 3
9.64903160E-10-2.81201547E-13-1.04006338E+03-4.13063173E+00
4

H2O H 2 O 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.23307477E+00-2.06131834E-03 5.50374416E-06-3.68298645E-09 8.79029373E-
13 2
-3.02934542E+04-1.00817640E+00 4.23307477E+00-2.06131834E-03 5.50374416E-
06 3
-3.68298645E-09 8.79029373E-13-3.02934542E+04-1.00817640E+00
4

H3N H 3 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.68574011E+00-2.93360885E-05 7.58342009E-06-6.30496036E-09 1.65518230E-
12 2
-6.50164988E+03 1.85952945E+00 3.68574011E+00-2.93360885E-05 7.58342009E-
06 3
-6.30496036E-09 1.65518230E-12-6.50164988E+03 1.85952945E+00
4

C2H4_Olef H 4 C 2 G 3.0E+02 1.5E+03 1.5E+03
1
8.53818289E-01 1.56513736E-02-4.17456118E-06-2.37439908E-09 1.22653109E-
12 2
5.40583073E+03 1.70030819E+01 8.53818289E-01 1.56513736E-02-4.17456118E-
06 3
-2.37439908E-09 1.22653109E-12 5.40583073E+03 1.70030819E+01
4

C2H6Nr_3 H 6 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.90670656E+00 2.57928715E-02-1.64499304E-05 5.88294130E-09-8.97151852E-
13 2

1.76112203E+04 1.12674688E+01 2.90670656E+00 2.57928715E-02-1.64499304E-
05 3
5.88294130E-09-8.97151852E-13 1.76112203E+04 1.12674688E+01
4

CHNHr H 2 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.38533457E+00 8.41863859E-03-3.69298455E-06 2.37797622E-10 2.02575843E-
13 2
3.17653719E+04 1.08394553E+01 2.38533457E+00 8.41863859E-03-3.69298455E-
06 3
2.37797622E-10 2.02575843E-13 3.17653719E+04 1.08394553E+01
4

C2H5r H 5 C 2 G 3.0E+02 1.5E+03 1.5E+03
1
1.79391466E+00 1.56170359E-02-2.65810195E-06-3.17752582E-09 1.31395465E-
12 2
1.32217198E+04 1.50609163E+01 1.79391466E+00 1.56170359E-02-2.65810195E-
06 3
-3.17752582E-09 1.31395465E-12 1.32217198E+04 1.50609163E+01
4

CH3N H 3 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.48021074E+00 4.79134432E-03 1.01312387E-05-1.18295083E-08 3.59462573E-
12 2
9.59014495E+03 1.13877890E+01 2.48021074E+00 4.79134432E-03 1.01312387E-
05 3
-1.18295083E-08 3.59462573E-12 9.59014495E+03 1.13877890E+01
4

C2H4Nr_3 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.77169114E+00 1.60072285E-02-3.85246304E-06-2.66303527E-09 1.27666059E-
12 2
2.75890673E+04 1.40471885E+01 2.77169114E+00 1.60072285E-02-3.85246304E-
06 3
-2.66303527E-09 1.27666059E-12 2.75890673E+04 1.40471885E+01
4

C2H4Nr_1 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
5.85381412E-01 2.72354440E-02-2.07768709E-05 8.52981842E-09-1.44925973E-
12 2
2.67695324E+04 1.88849515E+01 5.85381412E-01 2.72354440E-02-2.07768709E-
05 3
8.52981842E-09-1.44925973E-12 2.67695324E+04 1.88849515E+01
4

C2H5N_Olef H 5 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1

1.47260391E-01 3.04395408E-02-2.20995845E-05 8.45690929E-09-1.30117804E-
12 2
5.38740233E+03 2.33296666E+01 1.47260391E-01 3.04395408E-02-2.20995845E-
05 3
8.45690929E-09-1.30117804E-12 5.38740233E+03 2.33296666E+01
4

H2O2 H 2 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
3.21051847E+00 6.67259099E-03-2.58407953E-06-2.51390260E-10 3.22735841E-
13 2
-1.75267580E+04 7.95690884E+00 3.21051847E+00 6.67259099E-03-2.58407953E-
06 3
-2.51390260E-10 3.22735841E-13-1.75267580E+04 7.95690884E+00
4

Hr H 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.50166207E+00 5.68434189E-14-4.16333634E-16 4.33680869E-19-9.26442286E-
23 2
2.54738485E+04-4.56979496E-01 2.50166207E+00 5.68434189E-14-4.16333634E-
16 3
4.33680869E-19-9.26442286E-23 2.54738485E+04-4.56979496E-01
4

C2H6 H 6 C 2 G 3.0E+02 1.5E+03 1.5E+03
1
1.56231261E+00 1.53512743E-02 3.96592663E-06-9.34547220E-09 3.05066658E-
12 2
-1.12560290E+04 1.40034282E+01 1.56231261E+00 1.53512743E-02 3.96592663E-
06 3
-9.34547220E-09 3.05066658E-12-1.12560290E+04 1.40034282E+01
4

H2N_r H 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
4.05590523E+00-1.10580525E-03 4.20250538E-06-2.64249818E-09 5.55263493E-
13 2
2.20677623E+04 1.91432542E-01 4.05590523E+00-1.10580525E-03 4.20250538E-
06 3
-2.64249818E-09 5.55263493E-13 2.20677623E+04 1.91432542E-01
4

CH2CHN(S) H 3 C 2 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
4.14453572E+00 1.31731672E-02-6.28186453E-06 1.43989655E-09-1.30842159E-
13 2
4.85873563E+04 3.75755189E+00 3.85114887E-01 2.63155652E-02-2.31525336E-
05 3
1.07917240E-08-1.99497769E-12 4.94340048E+04 2.23684056E+01
4

C2H2Nr H 2 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.33489070E+00 1.75673299E-02-1.70392083E-05 9.50462024E-09-2.19183178E-
12 2
3.01115691E+04 1.19662075E+01 2.33489070E+00 1.75673299E-02-1.70392083E-
05 3
9.50462024E-09-2.19183178E-12 3.01115691E+04 1.19662075E+01
4

CH2Nr H 2 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.72280454E+00 5.87340845E-03 1.38451762E-06-3.57527614E-09 1.19017035E-
12 2
2.74896650E+04 9.64875177E+00 2.72280454E+00 5.87340845E-03 1.38451762E-
06 3
-3.57527614E-09 1.19017035E-12 2.74896650E+04 9.64875177E+00
4

C2H6Nr_1 H 6 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.07982204E+00 2.50240153E-02-1.20271968E-05 1.86154353E-09 2.23758117E-
13 2
1.72950463E+04 1.57761071E+01 2.07982204E+00 2.50240153E-02-1.20271968E-
05 3
1.86154353E-09 2.23758117E-13 1.72950463E+04 1.57761071E+01
4

HOrr H 1 O 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.49352200E+00 1.59367067E-04-7.68542411E-07 1.16517231E-09-4.05140241E-
13 2
3.46673516E+03 2.16823889E+00 3.49352200E+00 1.59367067E-04-7.68542411E-
07 3
1.16517231E-09-4.05140241E-13 3.46673516E+03 2.16823889E+00
4

Or O 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.50166207E+00 5.68434189E-14-4.16333634E-16 4.33680869E-19-9.26442286E-
23 2
2.92263414E+04 5.12365258E+00 2.50166207E+00 5.68434189E-14-4.16333634E-
16 3
4.33680869E-19-9.26442286E-23 2.92263414E+04 5.12365258E+00
4

CH3CN H 3 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.42890182E+00 1.39680388E-02-3.90817020E-06-1.61125025E-09 8.62317017E-
13 2
7.90367126E+03 1.13386705E+01 2.42890182E+00 1.39680388E-02-3.90817020E-
06 3
-1.61125025E-09 8.62317017E-13 7.90367126E+03 1.13386705E+01
4

HO2r H 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
3.31827958E+00 2.57325245E-03 1.65372177E-06-2.80836992E-09 9.38124626E-
13 2
3.66751518E+02 7.79640099E+00 3.31827958E+00 2.57325245E-03 1.65372177E-
06 3
-2.80836992E-09 9.38124626E-13 3.66751518E+02 7.79640099E+00
4

C2H6Nr_2 H 6 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.73186195E+00 2.74045777E-02-1.55148287E-05 3.83764212E-09-1.72831209E-
13 2
1.27543909E+04 1.70958608E+01 1.73186195E+00 2.74045777E-02-1.55148287E-
05 3
3.83764212E-09-1.72831209E-13 1.27543909E+04 1.70958608E+01
4

CH3r H 3 C 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.56490705E+00 4.13270098E-03-6.51104001E-07 1.23890293E-10-1.11133443E-
13 2
1.63675612E+04 1.91591164E+00 3.56490705E+00 4.13270098E-03-6.51104001E-
07 3
1.23890293E-10-1.11133443E-13 1.63675612E+04 1.91591164E+00
4

C2H4Nr_2 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
-4.72931344E-01 3.11386057E-02-2.65473994E-05 1.21955876E-08-2.29558493E-
12 2
2.38772229E+04 2.50494991E+01-4.72931344E-01 3.11386057E-02-2.65473994E-
05 3
1.21955876E-08-2.29558493E-12 2.38772229E+04 2.50494991E+01
4

CH4 H 4 C 1 G 3.0E+02 1.5E+03 1.5E+03
1
3.66148774E+00-2.55508829E-03 1.99198423E-05-1.70933764E-08 4.61455102E-
12 2
-1.00821382E+04 1.54144457E+00 3.66148774E+00-2.55508829E-03 1.99198423E-
05 3
-1.70933764E-08 4.61455102E-12-1.00821382E+04 1.54144457E+00
4

C2H5N_2 H 5 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.61611605E+00 1.90863164E-02-1.60307956E-06-6.21352712E-09 2.41625947E-
12 2
8.26503988E+03 1.72873068E+01 1.61611605E+00 1.90863164E-02-1.60307956E-
06 3

-6.21352712E-09 2.41625947E-12 8.26503988E+03 1.72873068E+01
4

c-C2H3N H 3 C 2 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
2.80979324E+00 1.50201816E-02-7.58141908E-06 1.85246807E-09-1.77642437E-
13 2
3.06581771E+04 8.95343001E+00 8.28524446E-02 2.20080656E-02-1.21834261E-
05 3
1.00059353E-09 1.01529601E-12 3.13995593E+04 2.30893128E+01
4

C2H3r_Olef H 3 C 2 G 3.0E+02 1.5E+03 1.5E+03
1
1.23353735E+00 1.69967037E-02-1.40402201E-05 6.83786802E-09-1.43151041E-
12 2
3.46975827E+04 1.65809399E+01 1.23353735E+00 1.69967037E-02-1.40402201E-
05 3
6.83786802E-09-1.43151041E-12 3.46975827E+04 1.65809399E+01
4

C2H4Nr_Olef_2 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.55148796E+00 2.47083115E-02-2.04141982E-05 9.60663180E-09-1.90057728E-
12 2
3.30064561E+04 1.82250407E+01 1.55148796E+00 2.47083115E-02-2.04141982E-
05 3
9.60663180E-09-1.90057728E-12 3.30064561E+04 1.82250407E+01
4

He He 1 G 3.0E+02 5.0E+03 1.0E+03
1
2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 2
-7.45686320E+02 9.08589239E-01 2.50104422E+00 0.00000000E+00
0.00000000E+00 3
0.00000000E+00 0.00000000E+00-7.45686320E+02 9.08589239E-01
4

O2 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
3.68638040E+00-2.12373381E-03 6.90709345E-06-6.01789533E-09 1.69609635E-
12 2
-1.05410485E+03 4.01804828E+00 3.68638040E+00-2.12373381E-03 6.90709345E-
06 3
-6.01789533E-09 1.69609635E-12-1.05410485E+03 4.01804828E+00
4

CH4Nr H 4 C 1 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.42329281E+00 2.01060190E-02-1.70458902E-05 8.48286639E-09-1.77547442E-
12 2

1.73273135E+04 1.61686751E+01 1.42329281E+00 2.01060190E-02-1.70458902E-
05 3
8.48286639E-09-1.77547442E-12 1.73273135E+04 1.61686751E+01
4

C2H7N H 7 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
9.81490707E-01 2.92684467E-02-1.28904982E-05 6.39604429E-10 8.01948302E-
13 2
-7.26886053E+03 2.01406012E+01 9.81490707E-01 2.92684467E-02-1.28904982E-
05 3
6.39604429E-10 8.01948302E-13-7.26886053E+03 2.01406012E+01
4

C2H4Nr_4 H 4 C 2 N 1 G 3.0E+02 1.5E+03 1.5E+03
1
2.49409783E+00 1.51256617E-02-6.42622674E-07-5.59996662E-09 2.12501276E-
12 2
2.24664753E+04 1.36887658E+01 2.49409783E+00 1.51256617E-02-6.42622674E-
07 3
-5.59996662E-09 2.12501276E-12 2.24664753E+04 1.36887658E+01
4

O3 O 3 G 2.0E+02 6.0E+03 1.0E+03
1
1.01625308E+01-7.76896990E-03 5.47843588E-06-1.22951829E-09 8.79720138E-
14 2
1.34525105E+04-2.90111737E+01 3.31673393E+00 2.68546939E-03 1.22411660E-
05 3
-2.07427723E-08 9.22985344E-12 1.58667815E+04 8.66105917E+00
4

CO O 1 C 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.03397274E+00 1.37328118E-03-4.96445087E-07 8.10281447E-11-4.85331749E-
15 2
-1.42586044E+04 6.10076092E+00 3.59508377E+00-7.21196937E-04 1.28238234E-
06 3
6.52429293E-10-8.21714806E-13-1.43448968E+04 3.44355598E+00
4

CO2 O 2 C 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.63537470E+00 2.74559459E-03-9.98282389E-07 1.61013606E-10-9.22018642E-
15 2
-4.90203677E+04-1.92887630E+00 2.20664321E+00 1.00970086E-02-9.96338809E-
06 3
5.47155623E-09-1.27733965E-12-4.83529864E+04 1.05261943E+01
4

CH2 C 1 H 2 G 2.0E+02 6.0E+03 1.0E+03
1

2.81412990E+00 3.79513443E-03-7.38424949E-07 7.19948955E-11-2.63188525E-
15 2
4.61859709E+04 6.52945537E+00 3.74842895E+00 1.07655977E-03 3.62462012E-
06 3
-4.46165519E-09 1.95224874E-12 4.58990472E+04 1.63509483E+00
4

CH2(S) C 1 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
2.86931299E+00 3.39756979E-03-1.00599964E-06 1.50562822E-10-8.61237607E-
15 2
5.06285244E+04 5.53163503E+00 4.18489675E+00-2.16396813E-03 7.68523621E-
06 3
-5.98243427E-09 1.67910304E-12 5.03923371E+04-7.17772105E-01
4

CH C 1 H 1 G 2.0E+02 6.0E+03 1.0E+03
1
2.74988924E+00 1.36248089E-03-2.71161485E-07 2.47828427E-11-1.18067699E-
15 2
7.08999411E+04 6.13979299E+00 3.49602032E+00 2.77423807E-04-1.57433829E-
06 3
3.07038632E-09-1.40468135E-12 7.06500301E+04 2.05802158E+00
4

C C 1 G 2.0E+02 6.0E+03 1.0E+03
1
2.60607421E+00-1.96384226E-04 1.06809851E-07-1.64080163E-11 8.15424248E-
16 2
8.54378446E+04 4.18935196E+00 2.55137539E+00-2.99926279E-04 6.79034717E-
07 3
-6.75577360E-10 2.46000780E-13 8.54693281E+04 4.54305445E+00
4

CH3OH O 1 C 1 H 4 G 2.0E+02 6.0E+03 1.0E+03
1
3.71775547E+00 1.00962072E-02-3.53785207E-06 5.61843105E-10-3.32714390E-
14 2
-2.60222319E+04 4.04182781E+00 5.52796377E+00-1.38922182E-02 6.21715706E-
05 3
-6.82045334E-08 2.52018995E-11-2.55968085E+04-7.15601292E-01
4

CH3O O 1 C 1 H 3 G 2.0E+02 6.0E+03 1.0E+03
1
4.75205127E+00 7.44944105E-03-2.70076415E-06 4.38793486E-10-2.64006093E-
14 2
4.44370836E+02-1.93362162E+00 3.71622806E+00-2.83500602E-03 3.77227316E-
05 3
-4.73647579E-08 1.86739253E-11 1.35874167E+03 6.55372649E+00
4

CH2OH O 1 C 1 H 3 G 2.0E+02 2.0E+03 1.0E+03
1
6.20503849E+00 2.43665952E-03 1.94377206E-06-1.61012603E-09 3.14355256E-
13 2
-4.25843527E+03-7.46070911E+00 4.40537005E+00-7.58358412E-04 2.61926168E-
05 3
-3.46319300E-08 1.40820009E-11-3.44228423E+03 3.60691223E+00
4

CH2O O 1 C 1 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
2.91332516E+00 6.70039926E-03-2.55520684E-06 4.27795142E-10-2.44072521E-
14 2
-1.44622358E+04 7.43822875E+00 4.77187231E+00-9.76266155E-03 3.70121918E-
05 3
-3.76921617E-08 1.31326646E-11-1.43798106E+04 6.96585679E-01
4

HCOH O 1 C 1 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
3.65237205E+00 5.55807060E-03-1.97617181E-06 3.16823378E-10-1.88747598E-
14 2
1.35536156E+04 4.22140840E+00 4.65733258E+00-9.53742306E-03 4.04679152E-
05 3
-4.45317569E-08 1.64761516E-11 1.38615127E+04 1.97860732E+00
4

HCO O 1 C 1 H 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.85781113E+00 2.64113950E-03-7.44177294E-07 1.23313230E-10-8.88958718E-
15 2
3.61642883E+03 3.92451197E+00 3.97074749E+00-1.49121608E-03 9.54041776E-
06 3
-8.82720349E-09 2.67645129E-12 3.84203291E+03 4.44660361E+00
4

HOCO O 2 C 1 H 1 G 2.0E+02 3.0E+03 1.0E+03
1
4.63988707E+00 5.66362726E-03-2.67855311E-06 6.17048884E-10-5.60953531E-
14 2
-2.40527335E+04 1.90175132E+00 2.82191157E+00 9.66218175E-03-2.78560177E-
06 3
-4.12692493E-09 2.61472072E-12-2.35465218E+04 1.14284719E+01
4

HOCHO O 2 C 1 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.61383160E+00 6.44963640E-03-2.29082510E-06 3.67160470E-10-2.18736750E-
14 2
-4.53303180E+04 8.47883830E-01 3.89836160E+00-3.55877950E-03 3.55205380E-
05 3
-4.38499590E-08 1.71077690E-11-4.67785744E+04 7.34953970E+00
4

OCHO O 2 C 1 H 1 N 0 G 3.0E+02 3.0E+03 1.0E+03
1
4.41052368E+00 7.50888367E-03-4.25889679E-06 1.12761124E-09-1.14144138E-
13 2
-1.70297531E+04 3.43148293E+00 3.62860375E+00 8.12496033E-03-1.41560718E-
06 3
-3.27951824E-09 1.61553900E-12-1.67477889E+04 7.83169538E+00
4

HOCH2O O 2 C 1 H 3 N 0 G 3.0E+02 3.0E+03 1.0E+03
1
3.64142330E+00 1.46738744E-02-8.24143161E-06 2.24789889E-09-2.38670785E-
13 2
-2.22304345E+04 7.15858335E+00-1.97308533E+00 4.26372227E-02-5.84444247E-
05 3
4.12218747E-08-1.13584932E-11-2.13827984E+04 3.28690136E+01
4

CH3OOH O 2 C 1 H 4 G 3.0E+02 3.0E+03 1.0E+03
1
4.45931439E+00 1.41050786E-02-6.53177245E-06 1.47662893E-09-1.32512049E-
13 2
-1.74300966E+04 4.03866676E+00 2.85836613E+00 1.59700646E-02-2.52104084E-
06 3
-5.73599921E-09 2.80534675E-12-1.68829666E+04 1.28970185E+01
4

CH3OO O 2 C 1 H 3 G 3.0E+02 3.0E+03 1.0E+03
1
2.88425280E+00 1.40067710E-02-6.88363514E-06 1.63789865E-09-1.53129010E-
13 2
-2.00432571E+01 1.18152986E+01 2.93065328E+00 8.68504133E-03 8.80315108E-
06 3
-1.39560866E-08 5.02939926E-12 2.27483038E+02 1.28754751E+01
4

CH2OOH O 2 C 1 H 3 G 2.0E+02 2.5E+03 1.0E+03
1
6.98746029E+00 9.00484259E-03-3.24366912E-06 5.24324826E-10-3.13587080E-
14 2
5.01257769E+03-1.02619220E+01 5.83126679E+00-3.51771199E-03 4.54550577E-
05 3
-5.66903320E-08 2.21633070E-11 6.06187060E+03-5.79143222E-01
4

C2H2 C 2 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.66165760E+00 4.88861739E-03-1.61257351E-06 2.48284097E-10-1.39736824E-
14 2
2.57695270E+04-4.01062351E+00 6.26263508E-01 2.47263532E-02-3.89555894E-
05 3

3.16484975E-08-9.87351295E-12 2.64555796E+04 1.46968104E+01
4

H2CC C 2 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.47847876E+00 4.84707787E-03-1.76213069E-06 2.92788093E-10-1.76554272E-
14 2
4.79490021E+04-7.84806167E-02 3.78897979E+00 5.91794674E-03-1.08086175E-
06 3
-1.85638085E-09 1.06887466E-12 4.81959632E+04 3.71766330E+00
4

C2H C 2 H 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.66270248E+00 3.82492252E-03-1.36632500E-06 2.13455040E-10-1.23216848E-
14 2
6.71683790E+04 3.92205792E+00 2.89867676E+00 1.32988489E-02-2.80733327E-
05 3
2.89484755E-08-1.07502351E-11 6.70616050E+04 6.18547632E+00
4

C2 C 2 G 2.0E+02 6.0E+03 1.0E+03
1
3.55870014E+00 7.86412096E-04-1.25558422E-07 8.97792994E-12-1.32453488E-
16 2
9.88903500E+04 4.18695466E+00 1.33654919E+00 3.59692890E-02-1.11849524E-
04 3
1.31762493E-07-5.29904082E-11 9.84220606E+04 9.54586591E+00
4

CH3CH2OH O 1 C 2 H 6 G 2.0E+02 6.0E+03 1.0E+03
1
6.56243650E+00 1.52042220E-02-5.38967950E-06 8.62250110E-10-5.12897870E-
14 2
-3.15256210E+04-9.47302020E+00 4.85869570E+00-3.74017260E-03 6.95553780E-
05 3
-8.86547960E-08 3.51688350E-11-2.99961320E+04 4.80185450E+00
4

CH3CHOH O 1 C 2 H 5 G 2.0E+02 6.0E+03 1.0E+03
1
6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-4.03713238E-
14 2
-9.53018581E+03-6.05106112E+00 4.22283250E+00 5.12174798E-03 3.48386522E-
05 3
-4.91943637E-08 2.01183723E-11-8.35622088E+03 8.01675700E+00
4

CH3CH2O O 1 C 2 H 5 G 2.0E+02 6.0E+03 1.0E+03
1
6.55053877E+00 1.32525511E-02-4.74726060E-06 7.64699226E-10-4.57008357E-
14 2

-4.47191998E+03-9.61231141E+00 3.26905655E+00 9.33562904E-03 2.96317166E-05 3
-4.53411341E-08 1.88795595E-11-2.95022955E+03 1.04200942E+01
4

CH2CH2OH O 1 C 2 H 5 G 2.0E+02 6.0E+03 1.0E+03
1
7.01348674E+00 1.20204391E-02-4.21992012E-06 6.70675981E-10-3.97135273E-14 2
-6.16161779E+03-8.62052409E+00 4.20954137E+00 9.12964578E-03 2.47462263E-05 3
-3.92945764E-08 1.66541312E-11-4.91511371E+03 8.30445413E+00
4

CH3CHO O 1 C 2 H 4 G 2.0E+02 6.0E+03 1.0E+03
1
5.40411080E+00 1.17230590E-02-4.22631370E-06 6.83724510E-10-4.09848630E-14 2
-2.25931220E+04-3.48079170E+00 4.72945950E+00-3.19328580E-03 4.75349210E-05 3
-5.74586110E-08 2.19311120E-11-2.15728780E+04 4.10301590E+00
4

CH2CHOH O 1 C 2 H 4 G 2.0E+02 6.0E+03 1.0E+03
1
7.49818166E+00 1.03957000E-02-3.66891058E-06 5.85205827E-10-3.47373827E-14 2
-1.81643092E+04-1.38388104E+01 2.28758479E+00 1.97013262E-02 1.96382662E-06 3
-1.94389758E-08 1.02616778E-11-1.65373421E+04 1.41333462E+01
4

cC2H4O O 1 C 2 H 4 G 2.0E+02 6.0E+03 1.0E+03
1
5.48876410E+00 1.20461900E-02-4.33369310E-06 7.00283110E-10-4.19490880E-14 2
-9.18042510E+03-7.07996050E+00 3.75905320E+00-9.44121800E-03 8.03097210E-05 3
-1.00807880E-07 4.00399210E-11-7.56081430E+03 7.84974750E+00
4

CHCHOH O 1 C 2 H 3 G 3.0E+02 6.0E+03 1.0E+03
1
8.78246275E+00 5.24796644E-03-1.71857235E-06 2.59722068E-10-1.48227402E-14 2
1.28836399E+04-2.10851258E+01-1.99180555E+00 4.73233467E-02-6.66058794E-05 3
4.68997052E-08-1.30686109E-11 1.52000823E+04 3.14259422E+01
4

cC2H3O O 1 C 2 H 3 G 2.0E+02 6.0E+03 1.0E+03
1

5.60158035E+00 9.17613962E-03-3.28028902E-06 5.27903888E-10-3.15362241E-
14 2
1.71446252E+04-5.47228512E+00 3.58349017E+00-6.02275805E-03 6.32426867E-
05 3
-8.18540707E-08 3.30444505E-11 1.85681353E+04 9.59725926E+00
4

CH2CHO O 1 C 2 H 3 G 2.0E+02 6.0E+03 1.0E+03
1
5.91636535E+00 8.84650426E-03-3.14954895E-06 5.05413189E-10-3.01304621E-
14 2
-1.04779892E+03-6.10649981E+00 2.66873956E+00 9.62329538E-03 1.60617438E-
05 3
-2.87681820E-08 1.25030066E-11 2.19438429E+02 1.25694476E+01
4

CH3CO O 1 C 2 H 3 G 2.0E+02 6.0E+03 1.0E+03
1
5.31371650E+00 9.17377930E-03-3.32203860E-06 5.39474560E-10-3.24523680E-
14 2
-3.64504140E+03-1.67575580E+00 4.03587050E+00 8.77294870E-04 3.07100100E-
05 3
-3.92475650E-08 1.52968690E-11-2.68207380E+03 7.86176820E+00
4

CH2CO O 1 C 2 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
5.75871449E+00 6.35124053E-03-2.25955361E-06 3.62321512E-10-2.15855515E-
14 2
-8.08533464E+03-4.96490444E+00 2.13241136E+00 1.81319455E-02-1.74093315E-
05 3
9.35336040E-09-2.01724844E-12-7.14808520E+03 1.33807969E+01
4

CHCHO O 1 C 2 H 2 G 2.0E+02 3.0E+03 1.0E+03
1
5.96287949E+00 7.99898746E-03-4.30605647E-06 1.11076174E-09-1.11415021E-
13 2
2.87255915E+04-5.17392496E+00 2.06863692E+00 1.87233234E-02-1.21318942E-
05 3
-3.33726595E-10 2.32881768E-12 2.97393543E+04 1.47865706E+01
4

HCCOH O 1 C 2 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
6.37509678E+00 5.49429011E-03-1.88136576E-06 2.93803536E-10-1.71771901E-
14 2
8.93277676E+03-8.24498007E+00 2.05541154E+00 2.52003372E-02-3.80821654E-
05 3
3.09890632E-08-9.89799902E-12 9.76872113E+03 1.22271534E+01
4

HCCO O 1 C 2 H 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.91479333E+00 3.71408730E-03-1.30137010E-06 2.06473345E-10-1.21476759E-
14 2
1.93596301E+04-5.50567269E+00 1.87607969E+00 2.21205418E-02-3.58869325E-
05 3
3.05402541E-08-1.01281069E-11 2.01633840E+04 1.36968290E+01
4

C2O O 1 C 2 G 2.0E+02 6.0E+03 1.0E+03
1
5.42468378E+00 1.85393945E-03-5.17932956E-07 6.77646230E-11-3.53315237E-
15 2
4.37161379E+04-3.69608405E+00 2.86278214E+00 1.19701204E-02-1.80851222E-
05 3
1.52777730E-08-5.20063163E-12 4.43125964E+04 8.89759099E+00
4

CH3CH2OOH O 2 C 2 H 6 G 2.0E+02 6.0E+03 1.0E+03
1
9.58691079E+00 1.48603589E-02-5.29787964E-06 8.47317148E-10-5.03436325E-
14 2
-2.38367900E+04-2.28310676E+01 4.14672004E+00 9.78668137E-03 4.91492257E-
05 3
-7.42532076E-08 3.11169441E-11-2.14671219E+04 9.84024999E+00
4

CH3CH2OO O 2 C 2 H 5 G 2.0E+02 6.0E+03 1.0E+03
1
8.88872432E+00 1.35833179E-02-4.91116949E-06 7.92343362E-10-4.73525704E-
14 2
-7.44107388E+03-1.90789836E+01 4.50099327E+00 6.87965342E-03 4.74143971E-
05 3
-6.92287127E-08 2.87395324E-11-5.39547911E+03 7.91490068E+00
4

CH3CHOOH O 2 C 2 H 5 G 2.0E+02 2.5E+03 1.0E+03
1
9.10837027E+00 1.52964186E-02-5.54863574E-06 9.02285762E-10-5.44120016E-
14 2
-9.32702959E+02-2.03914131E+01 6.26853790E+00 1.11351157E-04 6.15943537E-
05 3
-7.95035384E-08 3.12333450E-11 9.62571275E+02-1.80971233E-01
4

CH2CH2OOH O 2 C 2 H 5 G 2.0E+02 6.0E+03 1.0E+03
1
9.41379980E+00 1.33542122E-02-4.68067639E-06 7.43230845E-10-4.39824231E-
14 2
1.98459602E+03-2.24516643E+01 5.07456388E+00 1.32389561E-02 2.53758646E-
05 3
-4.38089546E-08 1.89061540E-11 3.71063204E+03 2.72289544E+00
4

CH2CHOOH O 2 C 2 H 4 G 1.0E+02 5.0E+03 1.0E+03
1
6.63483252E+00 1.21573021E-02-4.85358052E-06 9.00399479E-10-6.33053544E-
14 2
-1.78756952E+04-9.18287977E+00 3.04603315E+00 1.68249428E-02 1.90750325E-
06 3
-1.22901031E-08 5.28708738E-12-1.66468623E+04 1.06187228E+01
4

HOCH2CH2OO O 3 C 2 H 5 G 3.0E+02 2.5E+03 8.0E+02
1
5.56418200E-01 4.12518690E-02-3.10646870E-05 1.22929600E-08-1.99690710E-
12 2
-2.20473900E+04 2.49983080E+01 5.56418200E-01 4.12518690E-02-3.10646870E-
05 3
1.22929600E-08-1.99690710E-12-2.20473900E+04 2.49983080E+01
4

CH2CHOO O 2 C 2 H 3 G 3.0E+02 2.0E+03 1.0E+03
1
1.41603000E+00 2.99337210E-02-2.63851730E-05 1.17707090E-08-2.05115710E-
12 2
1.13617270E+04 1.89695260E+01 1.41461130E+00 2.97546290E-02-2.58393870E-
05 3
1.12220850E-08-1.86780970E-12 1.13712490E+04 1.90225610E+01
4

OCHCHO O 2 C 2 H 2 G 2.0E+02 6.0E+03 1.0E+03
1
8.72506895E+00 6.33096819E-03-2.35574814E-06 3.89782853E-10-2.37486912E-
14 2
-2.91024131E+04-2.03903909E+01 4.68412461E+00 4.78012819E-04 4.26390768E-
05 3
-5.79018239E-08 2.31669328E-11-2.71985007E+04 4.51187184E+00
4

OCHCO O 2 C 2 H 1 G 3.5E+02 2.9E+03 1.0E+03
1
4.94993880E+00 1.01630320E-02-5.57720100E-06 1.45720260E-09-1.47434750E-
13 2
-9.09650610E+03 2.57987980E+00 3.39405610E+00 1.43628560E-02-8.84137660E-
06 3
1.60961290E-09 3.20389380E-13-8.68414420E+03 1.05920410E+01
4

CH3C(O)OOH O 3 C 2 H 4 N 0 G 3.0E+02 3.0E+03 1.0E+03
1
5.64132391E+00 2.17230931E-02-1.11238026E-05 2.75682193E-09-2.67754066E-
13 2
-4.51408748E+04-1.61172400E+00 1.43747508E+00 3.39384339E-02-2.25467319E-
05 3

5.77205354E-09 1.28451673E-13-4.40701023E+04 1.98194302E+01
4

CH3C(O)OO O 3 C 2 H 3 N 0 G 3.0E+02 3.0E+03 1.0E+03
1
5.76603946E+00 1.88598136E-02-9.95181008E-06 2.52994204E-09-2.50541483E-
13 2
-2.21268244E+04-4.84080352E-01 2.12837736E+00 2.94919132E-02-2.00221362E-
05 3
5.32494396E-09 3.03452421E-14-2.12033645E+04 1.80451737E+01
4

CH3C(O)O O 2 C 2 H 3 N 0 G 3.0E+02 3.0E+03 1.0E+03
1
4.15456832E+00 1.68674623E-02-8.75191344E-06 2.18661448E-09-2.13394222E-
13 2
-2.52304326E+04 5.95052997E+00 1.30016170E+00 2.37699204E-02-1.23328477E-
05 3
5.87354833E-11 1.44736765E-12-2.44337929E+04 2.08501841E+01
4

NO O 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.25487317E+00 1.19869941E-03-4.33028500E-07 7.02943336E-11-4.09788575E-
15 2
9.90699836E+03 6.40395140E+00 4.08517990E+00-3.64693188E-03 8.49607612E-
06 3
-6.62405734E-09 1.77647373E-12 9.84061267E+03 2.83578236E+00
4

NH H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
2.79498941E+00 1.29259567E-03-3.85559094E-07 6.26027608E-11-3.70421913E-
15 2
4.23408998E+04 5.68413752E+00 3.45887003E+00 4.93904408E-04-1.87862560E-
06 3
2.85542239E-09-1.16864671E-12 4.21088372E+04 2.00373292E+00
4

N N 1 G 2.0E+02 6.0E+03 1.0E+03
1
2.41604245E+00 1.74663766E-04-1.18864562E-07 3.01850054E-11-2.03260159E-
15 2
5.61051512E+04 4.64905706E+00 2.49976643E+00 5.02149594E-07 1.93091211E-
09 3
-4.94632629E-12 2.74089506E-15 5.60760710E+04 4.19499326E+00
4

NNH H 1 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
3.42744423E+00 3.23295234E-03-1.17296299E-06 1.90508356E-10-1.14491506E-
14 2

2.88067740E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-
05 3
-1.33263744E-08 4.41023397E-12 2.88323793E+04 3.28551762E+00
4

N2H4 H 4 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.93957357E+00 8.75017187E-03-2.99399058E-06 4.67278418E-10-2.73068599E-
14 2
9.28265548E+03-2.69439772E+00 3.83472149E+00-6.49129555E-04 3.76848463E-
05 3
-5.00709182E-08 2.03362064E-11 1.00893925E+04 5.75272030E+00
4

N2H3 H 3 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.04483566E+00 7.31130186E-03-2.47625799E-06 3.83733021E-10-2.23107573E-
14 2
2.53241420E+04 2.88423392E+00 3.42125505E+00 1.34901590E-03 2.23459071E-
05 3
-2.99727732E-08 1.20978970E-11 2.58198956E+04 7.83176309E+00
4

N2H2 H 2 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
1.31115117E+00 9.00187208E-03-3.14911824E-06 4.81449581E-10-2.71897891E-
14 2
2.33863341E+04 1.64091067E+01 4.91066031E+00-1.07791880E-02 3.86516489E-
05 3
-3.86501698E-08 1.34852134E-11 2.28241901E+04 9.10273396E-02
4

H2NN H 2 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
3.05903670E+00 6.18382347E-03-2.22171165E-06 3.58539206E-10-2.14532905E-
14 2
3.48530149E+04 6.69893515E+00 4.53204001E+00-7.32418578E-03 3.00803713E-
05 3
-3.04000551E-08 1.04700639E-11 3.49580003E+04 1.51074195E+00
4

NH2OH O 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.88112502E+00 8.15708448E-03-2.82615576E-06 4.37930933E-10-2.52724604E-
14 2
-6.86018419E+03 3.79156136E+00 3.21016092E+00 6.19671676E-03 1.10594948E-
05 3
-1.96668262E-08 8.82516590E-12-6.58148481E+03 7.93293571E+00
4

H2NO O 1 H 2 N 1 G 2.0E+02 6.0E+03 1.0E+03
1

3.75555914E+00 5.16219354E-03-1.76387387E-06 2.75052692E-10-1.60643143E-
14 2
6.51826177E+03 4.30933053E+00 3.93201139E+00-1.64028165E-04 1.39161409E-
05 3
-1.62747853E-08 6.00352834E-12 6.71178975E+03 4.58837038E+00
4

HNOH O 1 H 2 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-
14 2
1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-
05 3
-3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00
4

HNO O 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.24129053E+00 2.72377193E-03-1.60633296E-07-9.79134982E-11 1.17103944E-
14 2
1.17745744E+04 7.27913637E+00 4.55326160E+00-5.84531688E-03 1.88853744E-
05 3
-1.76039893E-08 5.72889621E-12 1.16315603E+04 1.66850841E+00
4

HON O 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.12044656E+00 2.28738122E-03-7.14685362E-07 1.03332384E-10-5.70484100E-
15 2
2.43643963E+04 3.38857665E+00 4.15272450E+00-3.87826402E-03 2.05476031E-
05 3
-2.49049483E-08 9.87365462E-12 2.46037098E+04 4.56636321E+00
4

NO2 O 2 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.90482285E+00 2.14474498E-03-8.12654059E-07 1.55511957E-10-1.04113963E-
14 2
2.28958979E+03-2.33567018E-01 3.78712696E+00-4.29576834E-04 1.37383818E-
05 3
-1.74264140E-08 6.71249644E-12 2.89500124E+03 6.96592162E+00
4

HONO O 2 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.79144641E+00 3.64630732E-03-1.29112765E-06 2.06498233E-10-1.22138679E-
14 2
-1.15974343E+04-4.07145349E+00 3.16416438E+00 8.50517773E-03 5.48561573E-
07 3
-8.27656474E-09 4.39957151E-12-1.07744086E+04 1.00231941E+01
4

HNO2 O 2 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.66358504E+00 4.89854351E-03-1.79694193E-06 2.94420361E-10-1.78235577E-
14 2
-7.25216334E+03-3.06053640E-02 4.03779347E+00-4.46123109E-03 3.19440815E-
05 3
-3.79359490E-08 1.44570885E-11-6.53088236E+03 5.90620097E+00
4

NO3 O 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
7.37569146E+00 2.21733003E-03-5.75695789E-07 6.69775424E-11-2.58934700E-
15 2
6.22445577E+03-1.24945323E+01 3.35586850E+00 1.06545436E-02-2.86690494E-
06 3
-5.14711611E-09 3.08532286E-12 7.47534931E+03 8.94786516E+00
4

HONO2 O 3 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
8.03061257E+00 4.46368336E-03-1.72272779E-06 2.91611606E-10-1.80487362E-
14 2
-1.93033764E+04-1.62543421E+01 1.55975056E+00 2.01502169E-02-1.15217296E-
05 3
-2.31891230E-09 3.17580552E-12-1.73955871E+04 1.77294677E+01
4

N2O O 1 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
4.80641382E+00 2.65307443E-03-9.70797397E-07 1.62590150E-10-9.96738154E-
15 2
8.19798219E+03-2.10607801E+00 2.13942290E+00 1.21800874E-02-1.59189415E-
05 3
1.20920039E-08-3.85125915E-12 8.87008622E+03 1.12477534E+01
4

HNC C 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.17272154E+00 2.66569898E-03-8.92300150E-07 1.37331005E-10-7.95545718E-
15 2
2.17977474E+04 2.15196203E-01 2.36665269E+00 1.49943353E-02-3.03605651E-
05 3
2.99845678E-08-1.09094949E-11 2.19807517E+04 7.87287988E+00
4

CN C 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
3.73483746E+00 5.83996018E-05 2.90443997E-07-6.74403810E-11 4.33381923E-
15 2
5.17018679E+04 2.85162570E+00 3.62920077E+00-1.07172764E-03 2.42398215E-
06 3
-5.85516328E-10-3.75364456E-13 5.18668474E+04 3.91231279E+00
4

HNCO O 1 C 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.30045051E+00 4.02250821E-03-1.40962280E-06 2.23855342E-10-1.32499966E-
14 2
-1.61995274E+04-3.11770684E+00 2.24009031E+00 1.45600497E-02-1.54352330E-
05 3
8.55535028E-09-1.79631611E-12-1.54589951E+04 1.21663775E+01
4

HOCN O 1 C 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.28767714E+00 4.01746511E-03-1.40407465E-06 2.22562614E-10-1.31562375E-
14 2
-3.77409807E+03-2.64470976E+00 2.88943546E+00 1.16487242E-02-1.08005006E-
05 3
5.44138776E-09-1.06857286E-12-3.15296691E+03 9.51295652E+00
4

HCNO O 1 C 1 H 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.91979744E+00 4.00114600E-03-1.42063343E-06 2.27569621E-10-1.35504870E-
14 2
1.80385534E+04-8.26935223E+00 6.07949401E-01 2.82182431E-02-4.60451618E-
05 3
3.82559486E-08-1.23226501E-11 1.90714209E+04 1.69199098E+01
4

NCO O 1 C 1 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.08064474E+00 2.37443587E-03-9.07098904E-07 1.52286713E-10-9.31009234E-
15 2
1.35781204E+04-2.15734434E+00 2.77405177E+00 9.24523481E-03-9.91773586E-
06 3
6.68461303E-09-2.09520542E-12 1.42369570E+04 9.75458670E+00
4

NCN C 1 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
5.65711708E+00 1.64211333E-03-6.37923438E-07 1.11209213E-10-6.99328410E-
15 2
5.22097079E+04-6.14049950E+00 3.00703195E+00 8.38874126E-03-6.90466542E-
06 3
2.84868816E-09-5.74273041E-13 5.30044793E+04 7.78171011E+00
4

HNCN C 1 H 1 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
5.53846448E+00 3.89054126E-03-1.38104752E-06 2.21294765E-10-1.31827325E-
14 2
3.59635337E+04-3.39587098E+00 3.06754311E+00 1.06789939E-02-7.96224305E-
06 3

2.59883390E-09-1.27057612E-13 3.66623508E+04 9.41074995E+00

4

NCNO O 1 C 1 H 0 N 2 G 2.0E+02 3.0E+03 1.0E+03

1

3.99574293E+00 7.96025626E-06-5.76602969E-09 1.80395948E-12-2.08846880E-16 2

3.09883543E+04 8.58277153E+00 3.99833460E+00 8.03718093E-06-1.56383867E-08 3

1.20479659E-11-3.24908996E-15 3.09870621E+04 8.56707356E+00

4

NCNOH O 1 C 1 H 1 N 2 G 2.0E+02 3.0E+03 1.0E+03

1

4.69841132E+00 2.16546382E-03-1.81441347E-06 5.49591459E-10-5.89846481E-14 2

2.48820341E+04 4.04514611E+00 3.45317867E+00 4.03550194E-03 1.32583822E-06 3

-6.69960685E-09 3.42515650E-12 2.52609685E+04 1.07521087E+01

4

HNCNH C 1 H 2 N 2 G 3.0E+02 4.0E+03 1.5E+03

1

8.37414300E+00 2.36614300E-03-3.50232400E-07-4.39110200E-11 1.09685900E-14 2

1.46108800E+04-2.10739300E+01 1.00198500E+00 2.46401600E-02-2.75977000E-05 3

1.53247200E-08-3.26828000E-12 1.67936800E+04 1.69432500E+01

4

NCCN C 2 N 2 G 2.0E+02 6.0E+03 1.0E+03

1

6.70549520E+00 3.64271185E-03-1.30939702E-06 2.16421413E-10-1.31193815E-14 2

3.48824335E+04-1.04803146E+01 2.32928126E+00 2.61540993E-02-4.90009889E-05 3

4.61923035E-08-1.64325831E-11 3.56900732E+04 9.86348075E+00

4

CH3NO O 1 C 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03

1

5.04711802E+00 9.21544305E-03-3.29034831E-06 5.28940397E-10-3.15689858E-14 2

6.23718102E+03-7.74395570E-01 5.18534727E+00-6.34085575E-03 4.57171139E-05 3

-5.30421813E-08 1.99501601E-11 6.93771506E+03 2.18492659E+00

4

CH2NO O 1 C 1 H 2 N 1 G 2.0E+02 6.0E+03 1.0E+03

1

5.40281520E+00 6.90570010E-03-2.51629770E-06 4.10140660E-10-2.47183000E-14 2

2.45286900E+04-4.45742620E+00 3.87818580E+00-6.65308860E-03 5.39476100E-
05 3
-6.81768130E-08 2.71817460E-11 2.57168570E+04 7.46187740E+00
4

C2H5NO O 1 C 2 H 5 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
3.22313410E+00 2.51564380E-02-1.28735870E-05 3.18527380E-09-3.08950420E-
13 2
2.90561270E+03 9.66286460E+00 1.19503050E+00 2.84612030E-02-1.06192600E-
05 3
-3.12526110E-09 2.47059570E-12 3.55161590E+03 2.06492050E+01
4

CH3CHNO O 1 C 2 H 4 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
3.74754820E+00 2.12796520E-02-1.09796160E-05 2.73592160E-09-2.66953840E-
13 2
1.17411520E+04 7.08474550E+00 1.92228250E+00 2.44337260E-02-9.49024290E-
06 3
-2.40398310E-09 2.05476960E-12 1.23135540E+04 1.69273440E+01
4

CH2CHNO O 1 C 2 H 3 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
4.48740760E+00 1.70181590E-02-8.86194630E-06 2.23082720E-09-2.19836030E-
13 2
1.76460070E+04 2.34417250E+00 7.82133810E-01 2.86250950E-02-2.14511100E-
05 3
7.40944370E-09-7.10950300E-13 1.85477700E+04 2.10235160E+01
4

CHCHNO O 1 C 2 H 2 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
5.91529040E+00 1.21049980E-02-6.44647410E-06 1.65556870E-09-1.65982900E-
13 2
4.80915980E+04-3.57486610E+00 1.66767290E+00 2.79986070E-02-2.86415960E-
05 3
1.53554560E-08-3.31673950E-12 4.89959650E+04 1.71916480E+01
4

CH3NO2 O 2 C 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
6.73034758E+00 1.09601272E-02-4.05357875E-06 6.67102246E-10-4.04686823E-
14 2
-1.29143475E+04-1.01800883E+01 3.54053638E+00 1.86559899E-03 4.44946580E-
05 3
-5.87057133E-08 2.30684496E-11-1.11385976E+04 1.06884657E+01
4

CH2NO2 O 2 C 1 H 2 N 1 G 2.0E+02 6.0E+03 1.0E+03
1

7.57504807E+00 7.01471036E-03-2.51481162E-06 4.05670550E-10-2.42796598E-
14 2
1.23880080E+04-1.15985589E+01 2.42742248E+00 1.60496442E-02 2.84727836E-
06 3
-1.82218429E-08 9.35383557E-12 1.40120587E+04 1.61086425E+01
4

C2H5NO2 O 2 C 2 H 5 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
9.29092218E+00 1.61241540E-02-5.95122756E-06 9.76015021E-10-5.90147816E-
14 2
-1.73718622E+04-2.11218316E+01 4.43720206E+00 8.25501813E-03 5.01013815E-
05 3
-7.12335325E-08 2.88207797E-11-1.49913491E+04 9.09921108E+00
4

CH2CH2NO2 O 2 C 2 H 4 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
6.21841050E+00 2.20240260E-02-1.14710410E-05 2.88879660E-09-2.84836420E-
13 2
1.01421330E+04-3.01283140E+00 1.19814740E+00 3.83711550E-02-3.03908510E-
05 3
1.17680810E-08-1.57117670E-12 1.13328820E+04 2.21405170E+01
4

CH3CHNO2 O 2 C 2 H 4 N 1 G 3.5E+02 3.0E+03 1.0E+03
1
5.75402820E+00 2.29072910E-02-1.20613430E-05 3.06098840E-09-3.03460440E-
13 2
4.74588010E+03-5.60534260E-01 9.48311020E-01 3.73430400E-02-2.65342880E-
05 3
7.92249850E-09-3.22058090E-13 5.94637960E+03 2.38210530E+01
4

CH3ONO O 2 C 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
6.93605239E+00 9.97319424E-03-3.60642537E-06 5.83462161E-10-3.50058729E-
14 2
-1.08381899E+04-6.98144573E+00 6.15261387E+00-2.91937431E-03 4.14526828E-
05 3
-4.93954776E-08 1.85608328E-11-9.85260262E+03 8.04057190E-01
4

CH3ONO2 O 3 C 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
9.77845489E+00 1.10069541E-02-4.25928645E-06 7.18198185E-10-4.42041793E-
14 2
-1.88804487E+04-2.39163197E+01 3.91363583E+00 1.52137945E-02 1.73479131E-
05 3
-3.37074473E-08 1.44322204E-11-1.66103232E+04 9.44208392E+00
4

CH3CH2ONO O 2 C 2 H 5 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
9.21849299E+00 1.62001532E-02-5.98159944E-06 9.81277173E-10-5.93455530E-
14 2
-1.65544389E+04-1.88591687E+01 3.37137598E+00 1.37914267E-02 3.84687528E-
05 3
-6.02380553E-08 2.49654782E-11-1.40198744E+04 1.58650733E+01
4

CH3CH2ONO2 O 3 C 2 H 5 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
1.21360953E+01 1.70091385E-02-6.43739515E-06 1.07219880E-09-6.54950920E-
14 2
-2.41902070E+04-3.71640527E+01 3.75721604E+00 1.93623098E-02 3.87534117E-
05 3
-6.64089530E-08 2.82505579E-11-2.08444383E+04 1.11813240E+01
4

CH3CHNH O 0 C 2 H 5 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
1.99419246E+00 2.12775413E-02-1.02686597E-05 2.40039260E-09-2.20647891E-
13 2
4.56273305E+03 1.43228859E+01 2.24230513E+00 1.46071399E-02 8.25386853E-
06 3
-1.56259103E-08 5.70541553E-12 4.79700805E+03 1.45453734E+01
4

CHCHNH2 O 0 C 2 H 4 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
4.77534564E+00 1.46041683E-02-6.78153232E-06 1.55237043E-09-1.41604244E-
13 2
3.54379126E+04 3.02319529E-01 5.83297823E-01 3.10085354E-02-3.08423467E-
05 3
1.72290892E-08-3.96982789E-12 3.62945134E+04 2.06174831E+01
4

CHCNH2 O 0 C 2 H 3 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
4.67245309E+00 1.04989910E-02-4.62630454E-06 1.01345924E-09-8.92616681E-
14 2
2.60712723E+04-5.77430843E-01 1.34809615E+00 2.60893264E-02-3.14511691E-
05 3
2.11896099E-08-5.70652625E-12 2.66214983E+04 1.48874428E+01
4

CH2CNH O 0 C 2 H 3 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
4.08696039E+00 1.27930769E-02-6.17629436E-06 1.46135849E-09-1.36980402E-
13 2
2.06483281E+04 2.95368340E+00 6.74453393E-01 2.66535164E-02-2.72825709E-
05 3
1.57426210E-08-3.75989891E-12 2.13203089E+04 1.93644542E+01
4

CH2CHN(S)_m0 O 0 C 2 H 3 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
4.14453572E+00 1.31731672E-02-6.28186453E-06 1.43989655E-09-1.30842159E-
13 2
4.85873563E+04 3.75755189E+00 3.85114887E-01 2.63155652E-02-2.31525336E-
05 3
1.07917240E-08-1.99497769E-12 4.94340048E+04 2.23684056E+01
4

CHCNH O 0 C 2 H 2 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
5.54662620E+00 7.65157744E-03-3.57997666E-06 8.31108900E-10-7.71666875E-
14 2
4.53945633E+04-3.17646312E+00 2.87300918E+00 1.98561384E-02-2.41519574E-
05 3
1.60558556E-08-4.26087659E-12 4.58537821E+04 9.34467032E+00
4

H2NCHO O 1 C 1 H 3 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
4.93694660E+00 9.60834089E-03-3.32934933E-06 5.16597902E-10-2.99203362E-
14 2
-2.50910273E+04-2.00078185E+00 3.17952470E+00 1.94589990E-03 3.43329627E-
05 3
-4.64825836E-08 1.87268120E-11-2.40580400E+04 9.94755425E+00
4

H2NCO O 1 C 1 H 2 N 1 G 2.0E+02 6.0E+03 1.0E+03
1
5.69169331E+00 6.08717989E-03-2.09433522E-06 3.28448737E-10-1.92703890E-
14 2
-3.81028606E+03-3.22710215E+00 3.53640094E+00 9.73407134E-03-3.87292847E-
07 3
-5.90128176E-09 3.01181866E-12-3.09623872E+03 8.47952204E+00
4

CH3NHCH3 O 0 C 2 H 7 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
2.13913083E+00 2.68643078E-02-1.28763453E-05 2.99663495E-09-2.74772023E-
13 2
-4.17331872E+03 1.29759199E+01 1.22882380E+00 2.60430675E-02-4.95078244E-
06 3
-6.74954202E-09 3.27738931E-12-3.76813390E+03 1.84832422E+01
4

CH3NCH3 O 0 C 2 H 6 N 1 G 3.0E+02 3.0E+03 1.0E+03
1
1.54968373E+00 2.47836253E-02-1.20302906E-05 2.81641066E-09-2.58540173E-
13 2
1.73453147E+04 1.93447983E+01 3.61164557E+00 9.06653308E-03 2.27492150E-
05 3

-2.78391712E-08 9.27266651E-12 1.73063845E+04 1.12643356E+01
4

AR AR 1 G 2.0E+02 6.0E+03 1.0E+03
1
2.49989176E+00 1.56134837E-07-7.76108557E-11 1.52928085E-14-1.05304493E-
18 2
-7.45328403E+02 4.38029835E+00 2.49988611E+00 2.13037960E-07 8.97320772E-
10 3
-2.31395752E-12 1.30201393E-15-7.45354481E+02 4.38024367E+00
4

N2 N 2 G 2.0E+02 6.0E+03 1.0E+03
1
2.93802970E+00 1.41838030E-03-5.03281045E-07 8.07555464E-11-4.76064275E-
15 2
-9.17180990E+02 5.95521985E+00 3.53603521E+00-1.58270944E-04-4.26984251E-
07 3
2.37542590E-09-1.39708206E-12-1.04749645E+03 2.94603724E+00
4

! [_ SMILES="C(C(N(C(C([H])([H])[H])(O[O])[H])[H])([H])[H])([H])([H])[H]"
_]
! [_ INCHI="InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h4-5H,3H2,1-2H3/t4-/m1/s1"
_]

CCOOjNCC C 4 H 10 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
5.10360126E+00 4.48600927E-02-5.71932170E-06-1.46257244E-08 5.97025170E-
12 2
-9.76258924E+03 7.14980369E+00 5.10360126E+00 4.48600927E-02-5.71932170E-
06 3
-1.46257244E-08 5.97025170E-12-9.76258924E+03 7.14980369E+00
4

! [_ SMILES="C(C(N(C(C(O[O])([H])[H])([H])[H])[H])([H])[H])([H])([H])[H]"
_]
! [_ INCHI="InChI=1S/C4H10NO2/c1-2-5-3-4-7-6/h5H,2-4H2,1H3" _]

COOjCNCC C 4 H 10 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
2.28259795E+00 6.90641439E-02-5.90569750E-05 2.85148965E-08-5.82271241E-
12 2
-4.25353353E+03 2.00136246E+01 2.28259795E+00 6.90641439E-02-5.90569750E-
05 3
2.85148965E-08-5.82271241E-12-4.25353353E+03 2.00136246E+01
4

! [_ SMILES="C(C(N(C(C([H])([H])[H])([H])[H])O[O])([H])[H])([H])([H])[H]"
_]
! [_ INCHI="InChI=1S/C4H10NO2/c1-3-5(4-2)7-6/h3-4H2,1-2H3" _]

CCNOOjCC C 4 H 10 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
7.20333138E+00 4.12430710E-02-7.73935639E-06-1.03264553E-08 4.54383262E-
12 2

4.69606277E+03-3.18939250E+00 7.20333138E+00 4.12430710E-02-7.73935639E-06 3
-1.03264553E-08 4.54383262E-12 4.69606277E+03-3.18939250E+00
4

! [_ SMILES="C([C](N(C(C([H])([H])[H])(OO[H])[H])[H])([H])([H])[H]" _]
! [_ INCHI="InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h3-6H,1-2H3/t4-/m1/s1" _]
CCOONCjC C 4 H 10 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
-6.54517800E-02 9.16301507E-02-1.00668464E-04 5.78842642E-08-1.31228744E-11 2
-6.39607169E+03 2.82160463E+01-6.54517800E-02 9.16301507E-02-1.00668464E-04 3
5.78842642E-08-1.31228744E-11-6.39607169E+03 2.82160463E+01
4

! [_ SMILES="C(C([N]C(C([H])([H])[H])(OO[H])[H])([H])[H])([H])([H])[H]" _]
! [_ INCHI="InChI=1S/C4H10NO2/c1-3-5-4(2)7-6/h4,6H,3H2,1-2H3" _]
CCOONjCC C 4 H 10 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
-2.54308437E+00 8.80662351E-02-7.28508427E-05 2.70838145E-08-3.28667704E-12 2
-3.04278702E+03 4.06906527E+01-2.54308437E+00 8.80662351E-02-7.28508427E-05 3
2.70838145E-08-3.28667704E-12-3.04278702E+03 4.06906527E+01
4

! [_ SMILES="C(C(N=C(C([H])([H])[H])O[H])([H])[H])([H])([H])[H]" _]
! [_ INCHI="InChI=1S/C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,(H,5,6)" _]
CCdONCC C 4 H 9 N 1 O 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.07747138E+00 4.84711658E-02-2.03452895E-05-1.45568048E-09 2.31958242E-12 2
-3.42363559E+04 2.67177731E+01 1.07747138E+00 4.84711658E-02-2.03452895E-05 3
-1.45568048E-09 2.31958242E-12-3.42363559E+04 2.67177731E+01
4

! [_ SMILES="C(C(N=C=O)([H])[H])([H])([H])[H]" _]
! [_ INCHI="InChI=1S/C3H5NO/c1-2-4-3-5/h2H2,1H3" _]
OdCdNCC C 3 H 5 N 1 O 1 G 3.0E+02 1.5E+03 1.5E+03
1
1.21930748E+00 3.34130335E-02-1.82123546E-05 3.29956631E-09 2.91377304E-13 2
-1.83205809E+04 2.30865393E+01 1.21930748E+00 3.34130335E-02-1.82123546E-05 3
3.29956631E-09 2.91377304E-13-1.83205809E+04 2.30865393E+01
4

! [_ SMILES="C(C(N=C(OO[H])[H])([H])[H])([H])([H])[H]" _]
! [_ INCHI="InChI=1S/C3H7NO2/c1-2-4-3-6-5/h3,5H,2H2,1H3/b4-3-" _]
OOCdNCC C 3 H 7 N 1 O 2 G 3.0E+02 1.5E+03 1.5E+03
1
3.59531931E-01 4.29639260E-02-2.21011552E-05 2.56282638E-09 9.58670747E-13 2


```

! Hong et al., Proc. Comb. Inst. 33:309-316 (2011)
!
Or+H2=HOr+Hr
          3.80E+12    0.00 33.25 !
DUP
Or+H2=HOr+Hr
          8.80E+14    0.00 80.23 !
DUP

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
!
HOr+H2=Hr+H2O
          2.20E+08    1.51 14.35 !

! Michael and Sutherland, J. Phys. Chem. 92:3853 (1988)
!
!OH+OH=O+H2O
          1.4E07    1.689   -1167 !
! DUP
!OH+OH=O+H2O
          -2.7E10    0.567     0 !
! DUP
! M. Sangwan, L. N. Krasnoperov, J Phys Chem A 116 (2012) 11817-11822.
HOr+HOr=Or+H2O
          2.00E+07    1.65 2.64 !
DUP
HOr+HOr=Or+H2O
          2.60E+11   -0.06 -3.46 !
DUP

! HH: Refitted (400-3000 K) for better stability of the solvers (avoiding
negative 'A') 16-04-08
!
H2+M=Hr+Hr+M
          4.60E+19   -1.40 436.73    !
CO/  1.9/ CO2/  3.8/ H2/  2.5/ H2O/ 12.0/ AR/  0.0/
H2+AR=Hr+Hr+AR
          5.80E+18   -1.10 436.73    !

! Tsang and Hampson, J. Phys. Chem. Ref. Data, 15:1087 (1986)
!
Hr+Or+M=HOr+M
          4.70E+18   -1.00 0.00    !
CO/  1.9/ CO2/  3.8/ H2/  2.5/ H2O/ 12.0/ AR/  0.75/

! Tsang and Hampson, J. Phys. Chem. Ref. Data, 15:1087 (1986)
!
Or+Or+M=O2+M
          1.90E+13    0.00 -7.48 !
CO/  1.9/ CO2/  3.8/ H2/  2.5/ H2O/ 12.0/ AR/  0.0/

! Tsang W Hampson RF JPCRD 15:1087 1986
!
H2O+M=Hr+HOr+M
          6.10E+27   -3.32 505.39    !
CO/  1.9/ O2/  1.5/ CO2/  3.8/ H2/  3.0/ N2/  2.0/ H2O/ 0.0/

! Srinivasan and Michael, Int. J. Chem. Kinetic. 38 (2006)

```

! Rate constant is for Ar with efficiencies from Michael et al., J. Phys. Chem. A, 106 (2002)
! Efficiencies for CO and CO2 taken from Li et al., Int. J. Chem. Kinet. 36:566-575 (2004)
H2O+H2O=Hr+HOr+H2O

1.00E+26 -2.44 502.83 !

! Srinivasan and Michael, Int. J. Chem. Kinetic. 38 (2006)

! !

!=====
=====

! MAIN BATH GAS IS N2 (comment this reaction otherwise)

!

Hr+O2(+M)=HO2r(+M)

4.70E+12 0.44 0.00 !
LOW/ 6.37E+20 -1.72 2.20 /
TROE/ 0.5 1.0E-30 1.0E30 /
CO/ 1.9/ O2/ 0.78/ CO2/ 3.8/ H2/ 2.0/ H2O/ 14.0/ AR/ 0.67/

!=====
=====

! MAIN BATH GAS IS AR (comment this reaction otherwise)

!

!H+O2(+M)=HO2(+M) 4.7E12 0.440 0 !

! LOW/9.042E19 -1.50 4.922E02/
! TROE/0.5 1E-30 1E30/
! H2/3/ H2O/21/ O2/1.1/ CO/2.7/ CO2/5.4/ N2/1.5/

!=====
=====

! High-pressure limit from Troe, Proc. Comb. Inst. 28:1463-1469 (2000)
! Low-pressure limit from Michael et al., J. Phys. Chem. A 106:5297-5313
! Centering factors from Fernandes et al., Phys. Chem. Chem. Phys. 10:4313-4321 (2008)

!

HO2r+Hr=H2+O2

2.80E+06 2.09 -6.07 !

! Michael et al., Proc. Comb. Inst. 28:1471 (2000)

! Scaled by 0.75 Burke et al. (2012)

!

HO2r+Hr=HOr+HOr

7.10E+13 0.00 1.23 !

! Mueller et al., Int. J. Chem. Kinetic. 31:113 (1999)

!

HO2r+Hr=H2O+Or

1.40E+12 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

HO2r+Or=O2+HOr

2.90E+10 1.00 -3.03 !

! Fernandez-Ramos and Varandas, J. Phys. Chem. A 106:4077-4083 (2002)

! Scaled by 0.60 by Burke et al. 2012

!

$\text{HO}_2\text{r} + \text{HO}_\text{r} = \text{H}_2\text{O} + \text{O}_2$
 1.90E+20 -2.49 2.44 !
 DUP
 $\text{HO}_2\text{r} + \text{HO}_\text{r} = \text{H}_2\text{O} + \text{O}_2$
 1.20E+09 1.24 -5.48 !
 DUP
 ! M. P. Burke, S. J. Klippenstein, L. B. Harding, Proc Combust Inst 34
 (2013) 547-555.
 !
 $\text{HO}_2\text{r} + \text{HO}_2\text{r} = \text{H}_2\text{O}_2 + \text{O}_2$
 1.20E+09 0.77 -7.64 !
 DUP
 $\text{HO}_2\text{r} + \text{HO}_2\text{r} = \text{H}_2\text{O}_2 + \text{O}_2$
 1.30E+12 0.29 30.95 !
 DUP
 ! D. D. Y. Zhou, K. Han, P. Zhang, L. B. Harding, M. J. Davis, R. T.
 Skodje, J Phys Chem A 116 (2012) 2089-2100.
 !
 $\text{H}_2\text{O}_2 (+\text{M}) = \text{HO}_\text{r} + \text{HO}_\text{r} (+\text{M})$
 2.00E+12 0.90 203.97 !
 LOW/ 2.50E+24 -2.30 203.97 /
 TROE/ 0.43 1.0E-30 1.0E30 /
 CO/ 2.8/ O2/ 1.2/ CO2/ 1.6/ H2/ 3.7/ N2/ 1.5/ H2O/ 7.5/
 H2O2/ 7.7/ AR/ 1.0/

! Troe, Combust. Flame 158:594-601 (2011)
 ! Efficiencies for H2 and CO taken from Li et al., Int. J. Chem. Kinet.
 36:566-575 (2004)
 !
 $\text{H}_2\text{O}_2 + \text{H}_\text{r} = \text{H}_2\text{O} + \text{HO}_\text{r}$
 2.40E+13 0.00 16.61 !
 ! Tsang and Hampson, J. Phys. Chem. Ref. Data, 15:1087 (1986)
 !
 $\text{H}_2\text{O}_2 + \text{H}_\text{r} = \text{HO}_2\text{r} + \text{H}_2$
 4.80E+13 0.00 33.26 !
 ! Tsang and Hampson, J. Phys. Chem. Ref. Data, 15:1087 (1986)
 !
 $\text{H}_2\text{O}_2 + \text{O}_\text{r} = \text{HO}_2\text{r} + \text{HO}_\text{r}$
 9.60E+06 2.00 16.61 !
 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 $\text{H}_2\text{O}_2 + \text{HO}_\text{r} = \text{HO}_2\text{r} + \text{H}_2\text{O}$
 1.70E+12 0.00 1.33 !
 DUP
 $\text{H}_2\text{O}_2 + \text{HO}_\text{r} = \text{HO}_2\text{r} + \text{H}_2\text{O}$
 7.60E+13 0.00 30.42 !
 DUP
 ! Hong et al., J. Phys. Chem. A 114 (2010) 5718-5727
 !
 !

```

!
*****
****
!   CO/CO2 subset
*
!
*****
****
!
CO+Or (+M)=CO2 (+M)
      1.80E+10   0.00 9.97 !
LOW/   1.40E+24  -2.79 17.54 /
TROE/  1.0   1.0E-30   1.0E30   1.0E30   /
CO/    1.9/   CO2/  3.8/   H2/    2.5/   H2O/  12.0/

! Mueller MA Yetter RA Dryer FL IJCK 31:705 1999
!
CO+HOr=CO2+Hr
      8.70E+05   1.73 -2.87 !
PLOG/ 0.01315   2.10E+05   1.90 -4.45 /
PLOG/ 0.1315    2.50E+05   1.88 -4.36 /
PLOG/ 1.315    8.70E+05   1.73 -2.87 /
PLOG/ 13.158   6.80E+06   1.48 0.20 /
PLOG/ 131.58   2.30E+07   1.35 4.08 /

! J.P. Senosiain, S.J. Klippenstein, J.A. Miller, Proc. Combust. Inst. 30
(2005) 945-953.
!
CO+HOr=HOCO
      2.00E+20  -3.50 5.48 ! 1.0 atm interpolation - LPL
(JPS,SJK,&JAM 30th Symp)
PLOG/ 0.013158   1.70E+15  -2.68 3.59 /
PLOG/ 0.13158   5.90E+18  -3.35 3.71 /
PLOG/ 1.3158    2.60E+20  -3.50 5.48 /
PLOG/ 13.158    7.10E+20  -3.32 7.38 /
PLOG/ 131.58    1.10E+20  -2.78 8.60 /

! J.P. Senosiain, S.J. Klippenstein, J.A. Miller, Proc. Combust. Inst. 30
(2005) 945-953.
!
CO+HO2r=CO2+HOr
      1.60E+05   2.18 75.07 !

! You X Wang H Goos E Sung C-J Klippenstein SJ JCPA 111:4031-4042 2007
!
CO+O2=CO2+Or
      4.70E+12   0.00 253.13   !

! Bacskay GB Mackie JC JPCA 109:2019-2025 2005
!
CO+H2O2=HOCO+HOr
      3.60E+04   2.50 119.91   !

! P Glarborg P Marshall CPL 475 (2009) 40-43
!
HOCO (+M)=CO2+Hr (+M)
      8.20E+11   0.41 147.84   !
LOW/   6.00E+26  -3.15 155.29   /

```

TROE/ 0.39 1.0E-30 1.0E30 /

! DM Golden GP Smith AB McEwen C-L Yu B Eiteneer M Frenklach GL Vaghjiani
AR Ravishankara FP Tully J Phys Chem. A 102 (1998) 8598-8606.

!
HOCO+Hr=CO2+H2
3.10E+17 -1.35 2.32 !

! H.G. Yu, J.S. Francisco, J. Chem. Phys. 128 (2008) 244315.
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160 (300-
1000 K, fit).

!
HOCO+Hr=CO+H2O
6.00E+15 -0.53 8.89 !

! H.G. Yu, J.S. Francisco, J. Chem. Phys. 128 (2008) 244315.
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160 (300-
1000 K, fit).

!
HOCO+Or=CO2+HOr
9.00E+12 0.00 0.00 !

! H.G. Yu, J.T. Muckerman, J.S. Francisco, J. Chem. Phys. 127 (2007)
094302.

!
HOCO+HOr=CO2+H2O
4.60E+12 0.00 -0.37 !

DUP
HOCO+HOr=CO2+H2O
9.50E+06 2.00 -0.37 !

DUP

! Yu H-G Muckerman JT Francisco JS JPCA 109:5230-5236 2005

!
HOCO+HO2r=CO2+H2O2
4.00E+13 0.00 0.00 !

! H.G. Yu, G. Poggi, J.S. Francisco, J.T. Muckerman, J. Chem. Phys. 129
(2008) 214307.

!
HOCO+O2=CO2+HO2r
4.00E+09 1.00 0.00 !

! H.G. Yu, J.T. Muckerman, J. Phys. Chem. A 110 (2006) 5312-5316.
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160 (300-
1000 K, fit).

!
!
!

! CH2O subset

*

!

!

CH2O(+M)=HCO+Hr(+M)
 8.00E+15 0.00 367.05 !
 LOW/ 1.30E+36 -5.50 393.01 /

! Troe J JPCA 109:8320-8328 2005
 ! J. Troe, J. Phys. Chem. A 111 (2007) 3862-3867.
 !

CH2O(+M)=CO+H2(+M)
 3.70E+13 0.00 301.12 !
 LOW/ 4.40E+38 -6.10 393.01 /

! Troe J JPCA 109:8320-8328 2005
 ! J. Troe, J. Phys. Chem. A 111 (2007) 3862-3867.
 !

!CH2O+H=HCO+H2 5.9E03 3.130 1510 !
 ! Wang SK Dames EE Davidson DF Hanson RK, J. Phys. Chem. A 118 10201-
 10209 2014
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:

CH2O+Hr=HCO+H2
 1.40E+23 -2.35 73.30 ! 1 atm
 PLOG/ 0.04 7.40E+23 -2.73 68.53 /
 PLOG/ 1.0 1.40E+23 -2.35 73.30 /
 PLOG/ 10.0 7.30E+23 -2.67 73.78 /

DUP

CH2O+Hr=HCO+H2
 1.60E+15 -0.44 23.77 ! 1 atm
 PLOG/ 0.04 2.10E+10 1.06 15.56 /
 PLOG/ 1.0 1.60E+15 -0.44 23.77 /
 PLOG/ 10.0 4.20E+09 1.29 15.02 /

DUP

CH2O+Hr=Hr+CO+H2
 5.10E+07 2.18 48.22
 PLOG/ 0.04 7.20E+08 1.90 49.09 /
 PLOG/ 1.0 5.10E+07 2.18 48.22 /
 PLOG/ 10.0 1.10E+09 1.81 55.07 /

!

!CH2O+O=HCO+OH 4.2E11 0.570 2760 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:

CH2O+Or=HCO+HOr
 5.60E+31 -5.19 83.55

DUP

CH2O+Or=HCO+HOr
 1.40E+15 -0.53 16.78

DUP

CH2O+Or=Hr+CO+HOr
 2.50E+21 -1.90 94.87

!

!CH2O+OH=HCO+H2O 2.4E07 1.830 -1116 !
 ! S. Wang, D. F. Davidson, R. K. Hanson, Proc. Combust. Inst. 35 473-480
 2015
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:


```

CH2O+HOr=HCO+H2O
  1.90E+09  1.26 -1.26
  PLOG/ 0.04  3.60E+09  1.17 -0.86 /
  PLOG/ 1.0  1.90E+09  1.26 -1.26 /
  PLOG/ 10.0  1.10E+09  1.33 -1.64 /
CH2O+HOr=Hr+CO+H2O
  7.20E+10  0.89 38.95
  PLOG/ 0.04  7.00E+10  0.91 36.17 /
  PLOG/ 1.0  7.20E+10  0.89 38.95 /
  PLOG/ 10.0  8.40E+10  0.88 41.18 /

!
!CH2O+HO2=HCO+H2O2 4.1E04 2.500 10206 !
! Eiteneer B Yu CL Goldenberg M Frenklach M JPCA 102:5196 1998
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016:
!CH2O+HO2=HCO+H2O2 4.1E04 2.500 10206 !
! DUP
!CH2O+HO2=HCO+H2O2 -2.5E14 0.027 30133
! DUP
CH2O+HO2r=HCO+H2O2
  4.40E+08  1.30 50.75 ! refit
CH2O+HO2r=Hr+CO+H2O2
  2.50E+14  0.03 126.02

!
!CH2O+O2=HCO+HO2 2.4E05 2.500 36461 !
! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016:
!CH2O+O2=HCO+HO2 2.4E05 2.500 36461
! DUP
!CH2O+O2=HCO+HO2 -1.4E15 0.027 56388
! DUP
CH2O+O2=HCO+HO2r
  1.80E+16  -0.64 189.95 ! refit
DUP
CH2O+O2=HCO+HO2r
  6.60E+08  1.36 156.16 ! refit
DUP
CH2O+O2=Hr+CO+HO2r
  1.40E+15  0.03 235.93

!
HCO (+M)=Hr+CO (+M)
  4.90E+16  -0.93 82.53 !
  LOW/ 7.40E+21 -2.36 81.10 /
  TROE/ 0.103 139.0 10900.0 4550.0 /
  CO/ 1.5/ O2/ 1.5/ CO2/ 3.0/ H2/ 2.0/ N2/ 1.5/ He/ 1.3/
  H2O/ 15.0/ CH4/ 5.0/

! Yang et al., 8th U. S. National Combustion Meeting, 2013, 070RK-0163.
!
HCO+Hr=CO+H2
  1.10E+14  0.00 0.00 !

! Friedrichs G Herbon JT Davidson DF Hanson RK CPPC 4:5778-5788 2002

```

```

!
HCO+Or=CO+HOr
      3.00E+13   0.00 0.00  !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
Troee J Walker RW Warnatz J JPCRD 21:403 1992
!
HCO+Or=CO2+Hr
      3.00E+13   0.00 0.00  !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
Troee J Walker RW Warnatz J JPCRD 21:403 1992
!
HCO+HOr=CO+H2O
      1.10E+14   0.00 0.00  !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troee J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
!
!!HCO+O2=CO+HO2r
      6.90E+06   1.90 -5.73 !
HCO+O2=CO+HO2r
      7.580E+12   0.000      1.71      ! AramcoMech

! FassheberN Friedrichs G Marshall P Glarborg P J. Phys. Chem. A 119
(2015) 7305-7315.
!
HCO+HO2r=CO2+HOr+Hr
      3.00E+13   0.00 0.00  !

! Tsang W Hampson RF JPCRD 15:1087 1986
!
HCO+HCO=CO+CH2O
      2.70E+13   0.00 0.00  !

! Friedrichs G Herbon JT Davidson DF Hanson RK CPPC 4:5778-5788 2002
!
!
!
*****
****
!   CH4 subset
*
!
*****
****
!
CH3r+Hr (+M)=CH4 (+M)
      2.30E+14   0.03 0.60  !
LOW/   2.70E+35  -5.34 14.14 /
TROE/ 0.395 163.5 4250.3      1253676.0 /
CO/   1.4/ CO2/ 4.0/ H2/   4.0/ N2/   1.4/ H2O/ 10.0/ He/   2.0/
CH4/  3.85/ C2H6/ 4.5/ AR/   0.61/

! Sutherland JW Su M-C Michael JV IJCK 33:669-684 2001
!

```

$\text{CH}_4 + \text{O}_r = \text{CH}_3\text{r} + \text{H}_0\text{r}$
 4.40E+05 2.50 27.52 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 $\text{CH}_4 + \text{H}_0\text{r} = \text{CH}_3\text{r} + \text{H}_2\text{O}$
 1.00E+06 2.18 10.49 !
 ! Srinivasan NK Su M-C Sutherland JW Michael JV JPCA 109:7902-7914 2005
 !
 $\text{CH}_4 + \text{H}_02\text{r} = \text{CH}_3\text{r} + \text{H}_2\text{O}_2$
 4.70E+04 2.50 87.86 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 $\text{CH}_4 + \text{O}_2 = \text{CH}_3\text{r} + \text{H}_02\text{r}$
 2.00E+05 2.75 216.37
 ! $\text{CH}_3 + \text{H}_02 = \text{CH}_4 + \text{O}_2$ 1.2E05 2.228 3022 ! rv (not in
 paper)
 ! Srinivasan, Michael, Harding, Klippenstein, Combust Flame 149, 104
 (2007)
 !
 $\text{CH}_4 + \text{CH}_2 = \text{CH}_3\text{r} + \text{CH}_3\text{r}$
 4.30E+12 0.00 41.97 !
 ! Bohland T Dobe S Wagner HGg BBPC 89:1110 (1985)
 !
 $\text{CH}_4 + \text{CH}_2(\text{S}) = \text{CH}_3\text{r} + \text{CH}_3\text{r}$
 4.30E+13 0.00 0.00 !
 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 $\text{CH}_4 + \text{CH} = \text{C}_2\text{H}_4_{\text{Olef}} + \text{Hr}$
 3.00E+13 0.00 -1.67 !
 ! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
 Troe J Walker RW Warnatz J JPCRD 21:403 1992
 !
 $\text{CH}_3\text{r} + \text{M} = \text{CH} + \text{H}_2 + \text{M}$
 3.10E+15 0.00 338.36 !
 ! V Vasudevan, RK Hanson, DM Golden, CT Bowman, DF Davidson, J. Phys.
 Chem. A 2007, 111, 4062-4072
 !
 $\text{CH}_3\text{r} + \text{M} = \text{CH}_2 + \text{Hr} + \text{M}$
 2.20E+15 0.00 345.85 !
 ! V Vasudevan, RK Hanson, DM Golden, CT Bowman, DF Davidson, J. Phys.
 Chem. A 2007, 111, 4062-4072
 !
 $\text{CH}_3\text{r} + \text{Hr} = \text{CH}_2 + \text{H}_2$
 1.20E+06 2.43 49.96 !
 ! SJK unpublished; see P. Glarborg, J.A. Miller, B. Ruscic, S.J.
 Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68.

```

!
CH2(S)+H2=CH3r+Hr
      7.60E+13    0.00 0.00 ! #r

! P-F Lee, H Matsui, N-S Wang J. Phys. Chem. A 2012, 116, 1891-1896
!
CH3r+Or=CH2O+Hr
      6.90E+13    0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! Press JM Fockenberg C Flynn GW JPCA 104:6755-6763 2000 (82%)
!
CH3r+Or=H2+CO+Hr
      1.50E+13    0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! Press JM Fockenberg C Flynn GW JPCA 104:6755-6763 2000 (18%)
!
CH3r+HOr=CH2+H2O
      4.30E+04    2.57 16.72 !

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
! 300-3000 K abstraction on the triplet surface (not in paper)
!CH3+OH=CH2+H2O
      1.1E03    3.000    2780 !
! Wilson C Balint-Kurti GG JPCA 102:1625-1631 1998 (atm pres)
!
CH3r+HOr=CH3OH
      5.60E+30   -5.65 17.63 ! 1.3 atm
PLOG/ 0.001316    6.90E+30   -6.64 11.84 /
PLOG/ 0.013158    1.10E+32   -6.64 14.07 /
PLOG/ 0.131579    1.50E+32   -6.36 16.54 /
PLOG/ 1.315789    5.60E+30   -5.65 17.63 /
PLOG/ 13.157895   1.40E+27   -4.33 15.42 /
PLOG/ 131.578947  1.30E+22   -2.66 10.25 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!
!CH3OH(+M)=CH3+OH(+M)
      2.1E18   -0.6148  92540 !
! LOW /2.60E49 -8.80 101500/
! TROE /0.7656 1910 59.51 9374/
! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!
CH3r+HOr=CH2(S)+H2O
      4.30E+15   -0.86 7.90 ! 1.3 atm
PLOG/ 0.001316    1.10E+14   -0.46 -2.08 /
PLOG/ 0.013158    2.20E+14   -0.54 -0.92 /
PLOG/ 0.131579    1.20E+15   -0.73 2.51 /
PLOG/ 1.315789    4.30E+15   -0.86 7.90 /
PLOG/ 13.157895   4.40E+14   -0.54 12.27 /
PLOG/ 131.578947  6.10E+10    0.60 12.23 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!
CH3r+HOr=H2+CH2O
      3.60E+12   -0.53 8.54 ! 1.3 atm
PLOG/ 0.001316    3.90E+09    0.25 -5.11 /

```

PLOG/ 0.013158 2.00E+10 0.06 -2.61 /
PLOG/ 0.131579 2.80E+11 -0.25 2.08 /
PLOG/ 1.315789 3.60E+12 -0.53 8.54 /
PLOG/ 13.157895 2.20E+12 -0.43 14.29 /
PLOG/ 131.578947 2.40E+09 0.45 15.86 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!

CH3r+HOr=Hr+CH2OH

5.60E+10 0.74 16.61 ! 1.3 atm
PLOG/ 0.001316 8.40E+09 0.96 13.51 /
PLOG/ 0.013158 8.40E+09 0.96 13.51 /
PLOG/ 0.131579 1.00E+10 0.94 13.79 /
PLOG/ 1.315789 5.60E+10 0.74 16.61 /
PLOG/ 13.157895 5.50E+11 0.49 22.77 /
PLOG/ 131.578947 2.50E+10 0.91 26.79 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!

CH3r+HOr=Hr+CH3O

7.90E+08 1.06 49.62 ! 1.3 atm
PLOG/ 0.001316 7.90E+08 1.07 49.62 /
PLOG/ 0.013158 7.90E+08 1.07 49.62 /
PLOG/ 0.131579 7.90E+08 1.07 49.62 /
PLOG/ 1.315789 7.90E+08 1.06 49.62 /
PLOG/ 13.157895 1.00E+09 1.03 50.08 /
PLOG/ 131.578947 3.10E+09 0.92 54.31 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!

CH3r+HOr=H2+HCOH

6.50E+11 0.11 3.90 ! 1.3 atm
PLOG/ 0.001316 1.20E+09 0.83 -9.72 /
PLOG/ 0.013158 6.40E+09 0.63 -7.12 /
PLOG/ 0.131579 8.00E+10 0.34 -2.36 /
PLOG/ 1.315789 6.50E+11 0.11 3.90 /
PLOG/ 13.157895 2.10E+11 0.30 9.20 /
PLOG/ 131.578947 9.40E+07 1.29 10.14 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
! cis and trans products are combined as HCOH
!

CH3r+HO2r=CH3O+HOr

1.00E+12 0.27 -2.88 !

! Jasper, Klippenstein, Harding, Proc. Combust. Inst. 32, 279 (2009)
! OBS typo in H. Hashemi, J.M. Christensen, S. Gersen, H. Levinsky, S.J.
Klippenstein, P. Glarborg, Combust. Flame 172 (2016) 349-364 mechanism
(sign of E)
!

CH3r+O2=CH3O+Or

7.50E+12 0.00 118.39 !

! Srinivasan NK Su M-C Sutherland JW Michael JV JPCA 109:7902-7914 2005
!

CH3r+O2=CH2O+HOr

1.90E+11 0.00 41.18 !

! Srinivasan NK Su M-C Sutherland JW Michael JV JPCA 109:7902-7914 2005
!

CH3r+O2=CH3OO

	5.00E+22	-3.85	8.37	!	1 atm
PLOG/ 0.01	6.80E+24	-3.00	0.00	/	
PLOG/ 1.0	5.00E+22	-3.85	8.37	/	
PLOG/ 10.0	3.40E+21	-3.20	9.62	/	
PLOG/ 20.0	4.10E+20	-2.94	7.95	/	
PLOG/ 20.0	3.30E+29	-5.60	28.66	/	
PLOG/ 50.0	2.80E+18	-2.20	5.86	/	
PLOG/ 50.0	5.60E+28	-5.25	28.66	/	
PLOG/ 100.0	1.10E+19	-2.30	7.53	/	
PLOG/ 100.0	4.10E+30	-5.70	36.61	/	

! Fernandes RX Luther K Troe J JPCA 110:4442-4449 2006 (fit to data)

!

!CH2O+CH3=HCO+CH4 3.2E01 3.360 4310 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016:

!CH2O+CH3=HCO+CH4 3.2E01 3.360 4310

! DUP

!CH2O+CH3=HCO+CH4 -1.9E11 0.887 24237

! DUP

CH2O+CH3r=HCO+CH4

3.50E+05 2.16 26.08 ! refit

CH2O+CH3r=Hr+CO+CH4

1.90E+11 0.89 101.35

!

CH3r+HCO=CH4+CO

	1.80E+20	-2.30	20.00	!	1 atm
PLOG/ 0.05	2.90E+18	-1.84	8.93	/	
PLOG/ 0.1	8.70E+18	-1.97	11.23	/	
PLOG/ 1.0	1.80E+20	-2.30	20.00	/	
PLOG/ 10.0	1.10E+21	-2.45	31.03	/	

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J
Phys Chem A 2015, 119, 7724-7733.

!

CH3r+HCO=CH2CO+H2

	4.90E+08	0.75	3.52	!	1 atm
PLOG/ 0.05	6.10E+06	1.24	-7.25	/	
PLOG/ 0.1	1.10E+07	1.18	-5.45	/	
PLOG/ 1.0	4.90E+08	0.75	3.52	/	
PLOG/ 10.0	1.60E+11	0.11	18.36	/	

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J
Phys Chem A 2015, 119, 7724-7733.

!

!!CH3r+CH3r=C2H5r+Hr

5.40E+13 0.00 67.17 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH3r+CH2=C2H4_Olef+Hr
 1.20E+15 -0.34 0.64 !
 ! Jasper AW Klippenstein SJ Harding LB JPCA 111:8689-8707 2007
 !
 CH3r+CH2(S)=C2H4_Olef+Hr
 2.00E+13 0.00 0.00 !
 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH3r+CH=C2H3r_Olef+Hr
 3.00E+13 0.00 0.00 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !
 CH3r+C=C2H2+Hr
 5.00E+13 0.00 0.00 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !
 CH2+M=CH+Hr+M
 5.60E+15 0.00 372.38 !
 ! Bauerle S Klatt M Wagner HGg BBPC 99:870 1995
 !
 CH2+M=C+H2+M
 5.80E+12 0.50 286.60 !
 ! Bauerle S Klatt M Wagner HGg BBPC 99:870 1995
 !
 CH2+Hr=CH+H2
 1.60E+14 0.00 0.00 !
 ! See P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog.
 Energy Combust. Sci. 67 (2018) 31-68.
 !CH2+H=CH+H2 1.2E14 0.000 0 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH2+Or=CO+Hr+Hr
 1.20E+14 0.00 2.24 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH2+Or=CO+H2
 8.00E+13 0.00 2.24 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH2+HOr=CH2O+Hr
 2.80E+13 0.12 -0.67 !
 ! A.W. Jasper, S.J. Klippenstein, L.B. Harding, J. Phys. Chem. A 111
 (2007) 8699-8707.

!
 CH2+HOr=CH+H2O
 8.60E+05 2.02 28.35 !

! A.W. Jasper, S.J. Klippenstein, L.B. Harding, J. Phys. Chem. A 111
 (2007) 8699-8707.
 !

CH2+O2=CO2+Hr+Hr
 2.10E+09 0.99 -1.13 !

! SJK unpublished (2013)
 !

CH2+O2=CH2O+Or
 2.20E+09 1.08 5.00 ! #r

! SJK unpublished (2015), final value used in P. Glarborg, J.A. Miller,
 B. Ruscic, S.J. Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68
 !CH2+O2=CH2O+O 1.3E06 2.420 1604 !
 ! Preliminary value listed in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
 Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68
 !

CH2+CO2=CO+CH2O
 1.00E+11 0.00 4.18 !

! Glarborg P Miller JA Kee RJ CF 65:177 1986 est
 !

CH2+CH2=C2H2+Hr+Hr
 7.00E+13 0.00 0.03 !

! Jasper AW Klippenstein SJ Harding LB JPCA 111:8689-8707 2007
 !

CH2+CH2=C2H2+H2
 1.80E+13 0.00 0.03 !

! Jasper AW Klippenstein SJ Harding LB JPCA 111:8689-8707 2007
 !

CH2+CH=C2H2+Hr
 4.00E+13 0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !

CH2+C=C2H+Hr
 5.00E+13 0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !

CH2(S)+N2=CH2+N2
 1.30E+13 0.00 1.80 ! #r

! Hayes F Lawrance WD Staker WS King KD JPC 100:11314 1996 (N2)
 ! Typo in listing (E=400) in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
 Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68 !
 CH2(S)+AR=CH2+AR
 1.50E+13 0.00 3.70 !

! Hayes F Lawrance WD Staker WS King KD JPC 100:11314 1996

!
 CH2(S)+Hr=CH2+Hr
 2.00E+14 0.00 0.00 !

 ! JAM est
 !
 CH2(S)+Hr=CH+H2
 3.00E+13 0.00 0.00 !

 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH2(S)+Or=CO+Hr+Hr
 3.00E+13 0.00 0.00 !

 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH2(S)+HOr=CH2O+Hr
 3.00E+13 0.00 0.00 !

 ! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH2(S)+O2=CH2+O2
 3.10E+13 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH2(S)+H2O=CH2+H2O
 3.00E+13 0.00 0.00 !

 ! Hack W Wagner HGg Wilms A BBPC 92:620-627 1988
 ! Carstensen HH Wagner HGg BBPC 99:1539 1995
 !
 CH2(S)+CO2=CH2O+CO
 1.10E+13 0.00 0.00 !

 ! Koch M Temps FWagener R Wagner HGg BBPC 94:645-650
 !
 CH+Hr=C+H2
 1.20E+14 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH+Or=CO+Hr
 5.70E+13 0.00 0.00 !

 ! Messing I Filseth SV Sadowski CM Carrington T JCP 74:3874 1981
 !
 CH+HOr=HCO+Hr
 3.00E+13 0.00 0.00 !
 CH+HOr=Hr+CO+Hr
 1.80E+23 -2.47 83.37 !

 ! JAM est
 ! including prompt dissociation of HCO (following Labbe et al., J. Phys.
 Chem. Lett. 2016)
 !

$\text{CH} + \text{HOr} = \text{C} + \text{H}_2\text{O}$
4.00E+07 2.00 12.55 !

! JAM est
!
 $\text{CH} + \text{O}_2 = \text{HCO} + \text{Or}$
9.70E+13 0.00 0.00 !

$\text{CH} + \text{O}_2 = \text{Hr} + \text{CO} + \text{Or}$
2.00E+23 -2.47 83.37 !

! M. Rohrig E.L. Petersen D.F. Davidson R.K. Hanson C.T. Bowman, Int J
Chem Kinet 29 781-789 1997
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
 $\text{CH} + \text{H}_2\text{O} = \text{CH}_2\text{O} + \text{Hr}$
2.80E+07 1.59 -10.92 !

! SJK unpublished (2016)
!
 $\text{CH} + \text{CO}_2 = \text{HCO} + \text{CO}$
8.80E+06 1.75 -4.35 !

$\text{CH} + \text{CO}_2 = \text{Hr} + \text{CO} + \text{CO}$
5.30E+16 -0.72 79.02 !

! P Glarborg, LLB Bentzen, EF 22, 291-296 (2008)
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
 $\text{CH} + \text{CH}_2\text{O} = \text{CH}_2\text{CO} + \text{Hr}$
9.50E+13 0.00 -2.16 !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
Troe J Walker RW Warnatz J JPCRD 21:403 1992
! HMT Nguyen, HT Nguyen, T-N Nguyen, HV Hoang, L Vereecken J. Phys. Chem.
A 2014, 118, 8861-8871 (confirm major pr channel)
!
 $\text{C} + \text{HOr} = \text{CO} + \text{Hr}$
5.00E+13 0.00 0.00 !

! JAM est
!
 $\text{C} + \text{O}_2 = \text{CO} + \text{Or}$
2.00E+13 0.00 0.00 !

! Husain D Kirsch LJ Trans Faraday Soc 67:2025 1971
!
!
 $\text{CH}_3\text{OH} (+\text{M}) = \text{CH}_2 (\text{S}) + \text{H}_2\text{O} (+\text{M})$
3.10E+18 -1.02 383.72 !
LOW/ 5.40E+23 -8.34 416.71 /
TROE/ 0.9922 943.0 47310.0 47110.0 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007
!
 $\text{CH}_2\text{OH} + \text{Hr} (+\text{M}) = \text{CH}_3\text{OH} (+\text{M})$
4.30E+15 -0.79 0.00 !
LOW/ 3.84E+37 -6.21 5.58 /

TROE/ 0.25 210.0 1434.0 1.0E30 /

! GRI3.0
!
CH3O+Hr(+M)=CH3OH(+M)
2.40E+12 0.52 0.21 !
LOW/ 4.66E+41 -7.44 58.91 /
TROE/ 0.7 100.0 90000.0 10000.0 /
CO/ 1.5/ CO2/ 2.0/ H2/ 2.0/ N2/ 1.0/ H2O/ 6.0/ CH4/ 2.0/
C2H6/ 3.0/

! GRI3.0
!
CH3OH+Hr=CH2OH+H2
6.60E+04 2.73 18.61 !

! Moses JI Visscher C Fortney JJ Showman AP Lewis NK Griffith CA
Klippenstein SJ Shabram M Friedson AJ Marley MS Freedman RS Astrophys J
2011, 737, 15.
!
CH3OH+Hr=CH3O+H2
4.10E+04 2.66 38.58 !

! Moses JI Visscher C Fortney JJ Showman AP Lewis NK Griffith CA
Klippenstein SJ Shabram M Friedson AJ Marley MS Freedman RS Astrophys J
2011, 737, 15.
!
CH3OH+Or=CH2OH+HOr
2.10E+13 0.00 22.20 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! CL Rasmussen, KH Andersen, K Dam-Johansen, P Glarborg, IJCK 40, 423-441
(2008)
!
CH3OH+Or=CH3O+HOr
3.70E+12 0.00 22.20 ! (~15% est)

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! CL Rasmussen, KH Andersen, K Dam-Johansen, P Glarborg, IJCK 40, 423-441
(2008)
!
CH3OH+HOr=CH2OH+H2O
1.50E+08 1.44 0.47 !

! Srinivasan NK Su M-C Michael JV JPCA 111:3951-3958 2007
! CL Rasmussen, KH Andersen, K Dam-Johansen, P Glarborg, IJCK 40, 423-441
(2008)
!
CH3OH+HOr=CH3O+H2O
2.70E+07 1.44 0.47 !

! Srinivasan NK Su M-C Michael JV JPCA 111:3951-3958 2007
! CL Rasmussen, KH Andersen, K Dam-Johansen, P Glarborg, IJCK 40, 423-441
(2008)
!

$\text{CH}_3\text{OH} + \text{HO}_2\text{r} = \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$
 3.50E-04 4.85 43.29 !
 ! Alecu, I.M.; Truhlar, D.G. J Phys Chem A 2011, 115, 14599-14611.
 !
 $\text{CH}_3\text{OH} + \text{HO}_2\text{r} = \text{CH}_3\text{O} + \text{H}_2\text{O}_2$
 1.50E-03 4.61 66.64 !
 ! Alecu, I.M.; Truhlar, D.G. J Phys Chem A 2011, 115, 14599-14611.
 !
 $\text{CH}_3\text{OH} + \text{O}_2 = \text{CH}_2\text{OH} + \text{HO}_2\text{r}$
 3.60E+05 2.27 178.91 !
 ! Klippenstein SJ Harding LB Davis MJ Tomlin AS Skodje RT PCI 2011, 33,
 351-357.
 !
 $\text{CH}_3\text{O} + \text{HO}_2\text{r} = \text{CH}_3\text{OH} + \text{O}_2$
 1.40E+11 0.00 0.00 !
 ! Mousavipour, S. H.; Homayoon, Z. J Phys Chem A 2011, 115, 3291-3300.
 !
 $\text{CH}_3\text{OH} + \text{CH}_3\text{r} = \text{CH}_3\text{O} + \text{CH}_4$
 1.30E-02 4.16 25.11 ! T: 400-2000 K
 ! SJK in HASGLA15/CH4 (2016-06-03)
 $\text{CH}_3\text{O} + \text{CH}_4 = \text{CH}_3\text{OH} + \text{CH}_3$ 1.3E14 0.000 15073 !
 ! Wantuck PJ Oldenberg RC Baughcum SL Winn KR PCI 22:973-981 1988
 !
 $\text{CH}_3\text{OH} + \text{CH}_3\text{r} = \text{CH}_2\text{OH} + \text{CH}_4$
 7.40E-01 3.78 30.05 !
 ! Alecu and Truhlar, J Phys Chem A 115 (2011) 14599-14611
 !
 $\text{CH}_2\text{OH} (+\text{M}) = \text{CH}_2\text{O} + \text{Hr} (+\text{M})$
 7.40E+10 0.81 165.51 !
 LOW/ 3.50E+21 -1.99 100.34 /
 TROE/ 0.844 900.0 1.0 3315.0 /
 CO/ 1.5/ O2/ 1.0/ CO2/ 2.0/ H2/ 2.0/ CH2O/ 2.5/ He/ 0.67/
 H2O/ 6.0/ CH4/ 2.0/ AR/ 0.85/
 CH3OH/ 3.0/ C2H6/ 3.0/

! DamesGolden13
 !
 $\text{CH}_2\text{OH} = \text{CH}_2\text{O} + \text{H}$ 2.3E36 -7.530 44880 !
 ! PLOG/ 0.01 3.3E32 -7.180 39740/
 ! PLOG/ 0.1 8.3E41 -9.580 45730/
 ! PLOG/ 1.0 2.3E36 -7.530 44880/
 ! PLOG/ 20. 5.7E34 -6.640 46430/
 ! PLOG/ 50. 3.4E31 -5.570 45610/
 ! PLOG/ 100. 1.7E27 -4.210 44130/
 ! V Aranda JM Christensen MU Alzueta AD Jensen P Glarborg S Gersen Y Gao
 P Marshall, IJCK 45 (2013) 283-294.
 !
 $\text{CH}_2\text{OH} + \text{Hr} = \text{CH}_2\text{O} + \text{H}_2$
 4.00E+06 1.86 0.62 !
 ! XU K Xu ZF Lin MC Mol Phys 105:2763-2776 2007
 !

CH2OH+Or=CH2O+HOr
6.60E+13 0.00 -2.90 !

! Seetula JA Kalinovski IJ Slagle IR Gutman D Chem. Phys. Lett. 224:533
1994
!
CH2OH+HOr=CH2O+H2O
2.40E+13 0.00 0.00 !

! Tsang W JPCRD 16:471 1987
!
CH2OH+HO2r=CH2O+H2O2
1.20E+13 0.00 0.00 !

! Tsang W JPCRD 16:471 1987
!
CH2OH+O2=CH2O+HO2r
7.20E+13 0.00 15.63 !

DUP
CH2OH+O2=CH2O+HO2r
2.90E+16 -1.50 0.00 !

DUP

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
!
CH2OH+CH3r=C2H4_Olef+H2O
7.20E+29 -5.03 38.68 ! 1 atm
PLOG/ 0.001 6.30E+24 -3.71 11.71 /
PLOG/ 0.01 1.20E+25 -3.79 12.56 /
PLOG/ 0.1 3.20E+27 -4.45 22.36 /
PLOG/ 1.0 7.20E+29 -5.03 38.68 /
PLOG/ 10.0 1.70E+27 -4.18 46.66 /
PLOG/ 100.0 3.90E+17 -1.37 37.56 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455
!
CH2OH+HCO=CH3OH+CO
1.00E+13 0.00 0.00 !

! Tsang W JPCRD 16:471 1987
! Friedrichs G Herbon JT Davidson DF Hanson RK IJCK 36:157-169 2004
!
CH2OH+HCO=CH2O+CH2O
1.50E+13 0.00 0.00 !

! Tsang W JPCRD 16:471 1987
! Friedrichs G Herbon JT Davidson DF Hanson RK IJCK 36:157-169 2004
!
CH2OH+CH2O=CH3OH+HCO
5.50E+03 2.81 24.53 !
CH2OH+CH2O=CH3OH+Hr+CO
3.30E+13 0.34 107.90 !

! Tsang W JPCRD 16:471 1987
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)

```

!
CH2OH+CH2OH=CH3OH+CH2O
      4.80E+12    0.00 0.00 !

! Tsang W JPCRD 16:471 1987
!
CH2OH+CH3O=CH3OH+CH2O
      2.40E+12    0.00 0.00 !

! Tsang W JPCRD 16:471 1987
!
CH3O(+M)=CH2O+Hr(+M)
      1.10E+10    1.21 100.70 !
LOW/   6.00E+16  -0.55 75.36 /
TROE/  0.341 28.0 1000.0    2339.0 /
CO/    1.5/  O2/   1.0/  CO2/  2.0/  H2/   2.0/  CH2O/ 2.5/  He/   0.67/
H2O/   6.0/  CH4/   2.0/  AR/   0.85/
CH3OH/   3.0/  C2H6/ 3.0/

! DamesGolden13
!
!CH3O=CH2O+H          6.0E111 -31.120   64130 !
! PLOG/ 0.01          1.4E27  -5.990   27390/
! PLOG/ 0.1           2.3E16  -2.660   20860/
! PLOG/ 1.0           6.0E111 -31.120   64130/
! PLOG/ 20.           4.2E107 -29.490   63410/
! PLOG/ 50.           4.4E83  -22.090   53620/
! PLOG/ 100.          3.6E89  -23.640   57920/
! V Aranda JM Christensen MU Alzueta AD Jensen P Glarborg S Gersen Y Gao
P Marshall, IJCK 45 (2013) 283-294.
!
!CH3O=CH2OH          7.7E115 -32.100   63410 !
! PLOG/ 0.01          1.8E31  -6.960   26670/
! PLOG/ 0.1           2.9E20  -3.640   20140/
! PLOG/ 1.0           7.7E115 -32.100   63410/
! PLOG/ 20.           5.4E111 -30.460   62690/
! PLOG/ 50.           5.6E87  -23.060   52090/
! PLOG/ 100.          4.7E93  -24.610   57200/
! V Aranda JM Christensen MU Alzueta AD Jensen P Glarborg S Gersen Y Gao
P Marshall, IJCK 45 (2013) 283-294.
!
CH3O+Hr=CH2O+H2
      7.60E+08    1.50 -2.17 !

! XU K Xu ZF Lin MC Mol Phys 105:2763-2776 2007 (1 atm)
!
CH3O+Or=CH2O+HOr
      3.80E+12    0.00 0.00 !

! Ewig F Rhäsa D Zellner R Ber. Bunsenges. Phys. Chem. 91:708-717 1987
! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! (k/ktot=0.25[CEC05])
!
CH3O+HOr=CH2O+H2O
      1.80E+13    0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986

```

!
 CH3O+HO2r=CH2O+H2O2
 3.00E+11 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH3O+O2=CH2O+HO2r
 4.80E-01 3.57 -4.41 !

! V Aranda JM Christensen MU Alzueta AD Jensen P Glarborg S Gersen Y Gao
 P Marshall, IJCK 45 (2013) 283-294.
 !
 CH3O+CO=CH3r+CO2
 9.50E+25 -4.93 37.99 !

! Wang B Hou H Gu Y JPCA 103:8021-8029 1999 (1 bar,200-1000 K)
 !
 CH3O+CH3r=CH2O+CH4
 2.40E+13 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 CH3O+CH2O=CH3OH+HCO
 6.60E+11 0.00 9.56 !

! Fittschen, C.; Delcroix, B.; Gomez, N.; Devolder, P. J. Chim. Phys. 95
 2129-2142 1998
 !
 CH3O+CH3O=CH3OH+CH2O
 6.00E+13 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 !
 CH3OOH(+M)=CH3O+HOr(+M)
 4.10E+19 -1.15 185.04 !
 LOW/ 3.90E+42 -7.50 195.52 /
 TROE/ 0.8375 36562.0 498.8 9990.0 /

! A.W. Jasper, S.J. Klippenstein, L.B. Harding, Proc. Combust. Inst. 32
 (2009) 279-286.
 !
 CH3OOH+Hr=CH2OOH+H2
 5.40E+10 0.00 7.78 !

! Slemr F Warneck P IJCK 9:267 1977
 !
 CH3OOH+Hr=CH3OO+H2
 5.40E+10 0.00 7.78 !

! Slemr F Warneck P IJCK 9:267 1977
 !
 CH3OOH+Hr=CH3O+H2O
 1.20E+10 0.00 7.78 !

! Slemr F Warneck P IJCK 9:267 1977
 !

CH3OOH+Or=CH2OOH+HOr

1.60E+13 0.00 19.87 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH3OOH+Or=CH3OO+HOr

8.70E+12 0.00 19.87 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH3OOH+HOr=CH3OO+H2O

1.10E+12 0.00 -1.83 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH3OOH+HOr=CH2OOH+H2O

7.20E+11 0.00 -1.08 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH3OOH+HO2r=CH3OO+H2O2

4.10E+04 2.50 42.70 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807

! est CH2O+HO2=HCO+H2O2

!

CH3OO+Hr=CH3O+HOr

1.00E+14 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986

!

CH3OO+Or=CH3O+O2

2.90E+10 1.00 -3.03 !

! est HO2+O

!

CH3OO+HOr=CH3OH+O2

1.70E+14 0.00 0.00 !

! A. Bossolasco, E. P. Farago, C. Schoemaeker, C. Fittschen, Chem. Phys.
Lett. 593 (2014) 7-13

!

CH3OO+HO2r=CH3OOH+O2

2.50E+11 0.00 -6.23 !

! Tyndall GS Cox RA Granier C Lesclaux R Moortgat GK Pilling MJ
Ravishankara AR Wallington TJ J Geophys Res 106:12157-12182 2001

!

CH3OO+CH3r=CH3O+CH3O

5.10E+12 0.00 -5.90 !

! Keiffer M Miscampbell AJ Pilling MJ JCSFT2 84:505 1988

!

$\text{CH}_3\text{OOH} + \text{CH}_3\text{r} = \text{CH}_3\text{OO} + \text{CH}_4$
 1.60E-03 4.32 -0.98 !

! sjk/hashemi ch4
 !
 $\text{CH}_3\text{OO} + \text{CH}_2\text{OH} = \text{CH}_2\text{O} + \text{CH}_3\text{OOH}$
 1.20E+13 0.00 0.00 !

! est $\text{CH}_2\text{OH} + \text{HO}_2 = \text{CH}_2\text{O} + \text{H}_2\text{O}_2$
 !
 $\text{CH}_3\text{OO} + \text{HCO} = \text{CH}_3\text{O} + \text{Hr} + \text{CO}_2$
 3.00E+13 0.00 0.00 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est $\text{HCO} + \text{HO}_2 = \text{CO}_2 + \text{OH} + \text{H}$
 !
 $\text{CH}_3\text{OO} + \text{CO} = \text{CH}_3\text{O} + \text{CO}_2$
 1.60E+05 2.18 75.06 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est $\text{CO} + \text{HO}_2 = \text{CO}_2 + \text{OH}$
 !
 $\text{CH}_3\text{OO} + \text{CH}_2\text{O} = \text{CH}_3\text{OOH} + \text{HCO}$ 4.1E04 2.500 10206 !
 ! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est $\text{CH}_2\text{O} + \text{HO}_2 = \text{HCO} + \text{H}_2\text{O}_2$
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:
 $\text{CH}_3\text{OO} + \text{CH}_2\text{O} = \text{CH}_3\text{OOH} + \text{HCO}$
 4.10E+04 2.50 42.70 !
 $\text{CH}_3\text{OO} + \text{CH}_2\text{O} = \text{CH}_3\text{OOH} + \text{Hr} + \text{CO}$
 2.50E+14 0.03 126.08 !

!
 $\text{CH}_3\text{OO} + \text{CH}_3\text{O} = \text{CH}_2\text{O} + \text{CH}_3\text{OOH}$
 3.00E+11 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
 !
 $\text{CH}_3\text{OO} + \text{CH}_3\text{OH} = \text{CH}_3\text{OOH} + \text{CH}_2\text{OH}$
 4.00E+13 0.00 81.17 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est $\text{CH}_3\text{OH} + \text{HO}_2 = \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$
 !
 $\text{CH}_3\text{OO} + \text{CH}_3\text{OO} = \text{CH}_3\text{O} + \text{CH}_3\text{O} + \text{O}_2$
 1.10E+18 -2.40 7.53 !

DUP
 $\text{CH}_3\text{OO} + \text{CH}_3\text{OO} = \text{CH}_3\text{O} + \text{CH}_3\text{O} + \text{O}_2$
 7.00E+10 0.00 3.35 !

DUP

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 ! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 !
 $\text{CH}_3\text{OO} + \text{CH}_3\text{OO} = \text{CH}_3\text{OH} + \text{CH}_2\text{O} + \text{O}_2$
 2.00E+11 -0.55 -6.69 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH2OOH=CH2O+HOr
2.40E+12 -0.93 6.56 ! 1 atm
PLOG/ 0.04 9.60E+10 -0.93 6.56 /
PLOG/ 1.0 2.40E+12 -0.93 6.56 /
PLOG/ 10.0 2.50E+13 -0.93 6.61 /
PLOG/ 100.0 7.00E+14 -1.06 7.30 /

! Ing W-C Sheng CY Bozzelli JW FPT 83:111-145 2003

!
!
HCOH=CH2O
5.20E+13 0.00 134.34 ! kinf

! Xiong et al., Combust. Flame 161 (2014) 885-897

!
HCOH=CO+H2
6.60E+13 0.00 206.96 ! kinf

! Xiong et al., Combust. Flame 161 (2014) 885-897

!
HCOH+Hr=CH2O+Hr
1.00E+14 0.00 0.00 !

! est
!
HCOH+Hr=HCO+H2
2.00E+13 0.00 0.00 !

! est
!
HCOH+Hr=Hr+CO+H2
1.00E+13 0.00 0.00 !

! est
!
HCOH+Or=CO2+Hr+Hr
3.00E+13 0.00 0.00 !

! est
!
HCOH+HOr=HCO+H2O
2.00E+13 0.00 0.00 !

! est
!
HCOH+HOr=Hr+CO+H2O
1.00E+13 0.00 0.00 !

! est
!
CH2O+HOr=HOCH2O
6.30E+06 1.63 17.92

! Xu, et al., Int. J. Chem. Kinet. 38 (2006) 322-326

HOCH2O=HOCHO+Hr
1.00E+14 0.00 62.34

! S.J. Klippenstein, et al., Phys. Chem. Chem. Phys. 8 (2006) 1133-1147.
! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
!
!!C2H6+Hr=C2H5r+H2
7.40E+03 3.10 22.34 !

! S.L. Peukert, N.J. Labbe, R. Sivaramakrishnan, J.V. Michael, J. Phys.
Chem. A 117 (2013) 10228-10238 (500 - 2000 K)
!
C2H6+CH2(S)=C2H5r+CH3r
1.20E+14 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
!
C2H6+CH3OO=C2H5r+CH3OOH
1.90E+01 3.64 71.55 !

! Miller JA Klippenstein PCCP 6:1192-1202 2004
!
C2H5r+Hr(+M)=C2H6(+M)
5.20E+17 -0.99 6.61 !
LOW/ 1.99E+41 -7.08 27.97 /
TROE/ 0.8422 125.0 2219.0 6882.0 /
CO/ 1.5/ CO2/ 2.0/ H2/ 2.0/ N2/ 1.0/ H2O/ 6.0/ CH4/ 2.0/
C2H6/ 3.0/ AR/ 0.7/

! GRI3.0
! Stewart PH Rothem T Golden DM PCI 22:943-952
!
C2H5r+Or=CH3r+CH2O
4.20E+13 0.00 0.00 !

! Slagle IR Sarzynski D Gutman D Miller JA Melius CF JCSFT2 84:491 1988
!
C2H5r+Or=CH3CHO+Hr
5.30E+13 0.00 0.00 !

! Slagle IR Sarzynski D Gutman D Miller JA Melius CF JCSFT2 84:491 1988
!
C2H5r+Or=C2H4_Olef+HOr
3.10E+13 0.00 0.00 !

! Slagle IR Sarzynski D Gutman D Miller JA Melius CF JCSFT2 84:491 1988
!
C2H5r+HOr=C2H4_Olef+H2O
7.90E+22 -2.99 16.16 ! 1 atm
PLOG/ 0.001 1.30E+19 -1.96 1.14 /
PLOG/ 0.01 1.20E+19 -1.95 1.00 /
PLOG/ 0.1 4.10E+19 -2.10 2.62 /
PLOG/ 1.0 7.90E+22 -2.99 16.16 /
PLOG/ 10.0 2.80E+24 -3.33 32.42 /
PLOG/ 100.0 4.70E+18 -1.58 33.47 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

C2H5r+HO2r=CH3r+CH2OH

	6.50E+21	-2.35	25.20	!	1 atm
PLOG/	0.001	9.20E+17	-1.30	10.48	/
PLOG/	0.01	1.10E+18	-1.32	10.75	/
PLOG/	0.1	5.70E+18	-1.52	13.33	/
PLOG/	1.0	6.50E+21	-2.35	25.20	/
PLOG/	10.0	1.90E+25	-3.25	44.25	/
PLOG/	100.0	6.50E+22	-2.44	52.92	/

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

!!C2H5r+HO2r=CH3CH2O+HO2r

	3.10E+13	0.00	0.00	!
--	----------	------	------	---

! Ludwig W Brandt B Friedrichs G Temps F JPCA 110:3330-3337 2006

!

C2H5r+O2=CH3CH2OO

	4.00E+42	-9.86	33.99	!	1 atm
PLOG/	1.0E-4	1.30E+42	-11.12	21.49	/
PLOG/	3.0E-4	2.00E+43	-11.30	22.95	/
PLOG/	0.001	1.20E+44	-11.36	24.48	/
PLOG/	0.003	3.20E+44	-11.32	25.93	/
PLOG/	0.01	1.30E+45	-11.33	28.29	/
PLOG/	0.03	1.20E+45	-11.15	29.97	/
PLOG/	0.1	4.30E+44	-10.83	31.65	/
PLOG/	0.3	4.90E+43	-10.37	32.68	/
PLOG/	1.0	4.00E+42	-9.86	33.99	/
PLOG/	3.0	1.20E+40	-8.95	32.87	/
PLOG/	10.0	2.20E+37	-7.95	31.48	/
PLOG/	30.0	1.60E+34	-6.88	28.92	/
PLOG/	100.0	1.60E+30	-5.56	24.72	/

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H5r+O2=C2H4_Olef+HO2r

	2.50E+09	0.51	4.84	
PLOG/	1.0E-4	9.10E+00	2.87	-21.33 /
PLOG/	3.0E-4	1.20E+01	2.84	-21.04 /
PLOG/	0.001	2.80E+01	2.73	-20.00 /
PLOG/	0.003	1.10E+02	2.56	-18.33 /
PLOG/	0.01	9.60E+02	2.30	-15.63 /
PLOG/	0.03	1.30E+04	1.98	-12.27 /
PLOG/	0.1	4.90E+05	1.54	-7.49 /
PLOG/	0.3	2.40E+07	1.07	-2.08 /
PLOG/	1.0	2.50E+09	0.51	4.84 /
PLOG/	3.0	1.40E+11	0.04	11.67 /
PLOG/	10.0	3.10E+12	-0.31	18.83 /
PLOG/	30.0	5.30E+12	-0.33	23.97 /
PLOG/	100.0	1.90E+11	0.14	26.66 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H5r+O2=CH2CH2OOH

	3.60E+26	-6.03	23.91	!	1 atm
--	----------	-------	-------	---	-------

PLOG/ 1.0E-4 3.20E+21 -5.53 -0.35 /
 PLOG/ 3.0E-4 4.60E+23 -6.12 2.45 /
 PLOG/ 0.001 2.90E+25 -6.60 5.35 /
 PLOG/ 0.003 2.90E+24 -6.19 5.14 /
 PLOG/ 0.01 5.90E+25 -6.49 8.48 /
 PLOG/ 0.03 2.90E+25 -6.26 10.25 /
 PLOG/ 0.1 4.60E+26 -6.47 15.05 /
 PLOG/ 0.3 4.70E+26 -6.29 18.90 /
 PLOG/ 1.0 3.60E+26 -6.03 23.91 /
 PLOG/ 3.0 6.30E+25 -5.58 28.42 /
 PLOG/ 10.0 6.60E+23 -4.74 32.45 /
 PLOG/ 30.0 7.70E+20 -3.63 34.81 /
 PLOG/ 100.0 1.90E+15 -1.72 33.61 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H5r+O2=cC2H4O+HO_r

 4.10E+00 2.65 -8.07 ! 1 atm
 PLOG/ 1.0E-4 1.40E-05 4.20 -23.51 /
 PLOG/ 3.0E-4 1.90E-05 4.16 -23.17 /
 PLOG/ 0.001 5.00E-05 4.04 -22.01 /
 PLOG/ 0.003 2.30E-04 3.85 -20.19 /
 PLOG/ 0.01 2.60E-03 3.55 -17.24 /
 PLOG/ 0.03 5.20E-02 3.18 -13.55 /
 PLOG/ 0.1 4.10E+00 2.65 -8.07 /
 PLOG/ 0.3 6.10E+02 2.04 -1.55 /
 PLOG/ 1.0 4.90E+05 1.22 7.54 /
 PLOG/ 3.0 5.00E+08 0.39 17.65 /
 PLOG/ 10.0 8.80E+11 -0.49 30.08 /
 PLOG/ 30.0 1.70E+14 -1.09 41.57 /
 PLOG/ 100.0 9.70E+14 -1.22 52.30 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H6+HCO=C2H5r+CH2O

 2.30E+00 3.74 70.85 !

! Huynh L.K.; Truong T.N. Theor. Chem. Acct. 120 (2008) 107-118

!C2H5+CH2O=C2H6+HCO 5.5E03 2.810 5860 !

! Tsang W Hampson RF JPCRD 15:1087 1986

!

C2H5r+HCO=C2H6+CO

 4.30E+13 0.00 0.00 !

! Baggott, J.E.; Frey, H.M.; Lightfoot, P.D.; Walsh, R. J. Phys. Chem. 91 (1987) 3386

!

C2H5r+HCO=CH3r+CH2CHO

 6.50E+21 -2.35 25.20 ! 1 atm
 PLOG/ 0.001 9.20E+17 -1.30 10.48 /
 PLOG/ 0.01 1.10E+18 -1.32 10.75 /
 PLOG/ 0.1 5.70E+18 -1.52 13.33 /
 PLOG/ 1.0 6.50E+21 -2.35 25.20 /
 PLOG/ 10.0 1.90E+25 -3.25 44.25 /
 PLOG/ 100.0 6.50E+22 -2.44 52.92 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!
 C2H5r+CH3r=C2H4_Olef+CH4
 9.00E+11 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

C2H5r+CH3OO=CH3CH2O+CH3O
 5.10E+12 0.00 -5.90 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est CH3OO+CH3=CH3O+CH3O
 !

C2H5r+C2H5r=C2H6+C2H4_Olef
 1.50E+12 0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
 Troe J Walker RW Warnatz J JPCRD 21:403 1992
 !

C2H3r_Olef+Hr(+M)=C2H4_Olef(+M)
 3.90E+13 0.20 0.00 !
 LOW/ 2.10E+24 -1.30 0.00 /
 TROE/ 0.5 1.0E-30 1.0E30 1.0E30 /

! Harding LB Georgievskii Y Klippenstein SJ JPCA 109:4646-4656 2005
 ! Monks PS Nesbitt FL Payne WA Scanlon M Stief LJ Shallcross DE JPC
 99:17151-17159 1995
 !

C2H4_Olef(+M)=H2CC+H2(+M)
 8.00E+12 0.44 371.54 !
 LOW/ 7.00E+50 -9.31 417.98 /
 TROE/ 0.735 180.0 1035.0 5417.0 /
 H2O/ 6.0/ AR/ 0.7/

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

C2H4_Olef+Or=CH3r+HCO
 5.90E+17 -1.72 12.10 !

C2H4_Olef+Or=CH3r+Hr+CO
 3.50E+27 -4.19 95.47 !

! Li, Jasper, Zador, Miller, Klippenstein, Proc. Combust. Inst. (2016)
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:
 !

C2H4_Olef+Or=CH3CO+Hr
 8.70E+12 -0.48 8.19 !

! Li, Jasper, Zador, Miller, Klippenstein, Proc. Combust. Inst. (2016)
 !

C2H4_Olef+Or=CH2CHO+Hr
 9.20E+09 0.95 7.21 !

! Li, Jasper, Zador, Miller, Klippenstein, Proc. Combust. Inst. (2016)
 !

C2H4_Olef+Or=CH2+CH2O
 5.80E+06 1.99 11.96 !

! Li, Jasper, Zador, Miller, Klippenstein, Proc. Combust. Inst. (2016)

!

C2H4_Olef+Or=CH2CO+H2

1.10E+17 -1.83 13.29 !

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

!

C2H4_Olef+HOr=CH3r+CH2O

1.80E+05 1.68 8.62 ! 1 atm
PLOG/ 0.01 5.40E+00 2.92 -7.25 /
PLOG/ 0.025 3.20E+01 2.71 -4.90 /
PLOG/ 0.1 5.60E+02 2.36 -0.76 /
PLOG/ 1.0 1.80E+05 1.68 8.62 /
PLOG/ 10.0 2.40E+09 0.56 25.13 /
PLOG/ 100.0 2.80E+13 -0.50 47.93 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

!

C2H4_Olef+HOr=CH3CHO+Hr

2.40E-02 3.91 7.21 ! 1 atm
PLOG/ 0.01 2.40E-07 5.30 -8.58 /
PLOG/ 0.025 8.70E-05 4.57 -2.59 /
PLOG/ 0.1 4.00E-01 3.54 7.87 /
PLOG/ 1.0 2.40E-02 3.91 7.21 /
PLOG/ 10.0 8.30E+08 1.01 43.96 /
PLOG/ 100.0 6.80E+09 0.81 58.02 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

!

C2H4_Olef+HOr=CH2CHOH+Hr

3.20E+05 2.19 21.99 ! 1 atm
PLOG/ 0.01 1.00E+04 2.60 17.24 /
PLOG/ 0.025 1.10E+04 2.60 17.28 /
PLOG/ 0.1 1.50E+04 2.56 17.73 /
PLOG/ 1.0 3.20E+05 2.19 21.99 /
PLOG/ 10.0 1.90E+08 1.43 32.76 /
PLOG/ 100.0 8.60E+10 0.75 48.08 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

!

C2H4_Olef+HOr=CH2CH2OH

6.00E+37 -8.14 33.65 ! 1 atm
PLOG/ 0.01 1.40E+47 -11.64 46.44 /
PLOG/ 0.025 6.00E+37 -9.76 8.35 /
PLOG/ 0.1 6.00E+37 -9.65 9.89 /
PLOG/ 1.0 6.00E+37 -8.14 33.65 /
PLOG/ 10.0 6.00E+37 -7.77 44.92 /
PLOG/ 100.0 6.00E+37 -7.44 59.70 /

DUP

C2H4_Olef+HOr=CH2CH2OH

7.30E+31 -6.91 11.95 ! 1 atm
PLOG/ 0.01 1.40E+47 -11.64 46.44 /
PLOG/ 0.025 5.00E+37 -8.68 22.41 /
PLOG/ 0.1 2.60E+35 -7.79 20.99 /
PLOG/ 1.0 7.30E+31 -6.91 11.95 /
PLOG/ 10.0 3.00E+26 -4.87 9.61 /
PLOG/ 100.0 2.80E+19 -2.41 4.23 /

DUP

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

!

C2H4_Olef+HO2r=CH2CH2OOH

2.70E+29 -6.27 73.35 ! 1 atm
PLOG/ 1.0E-4 3.10E+20 -5.24 46.15 /
PLOG/ 3.0E-4 2.70E+20 -5.14 47.82 /
PLOG/ 0.001 2.60E+21 -5.24 51.00 /
PLOG/ 0.003 1.20E+23 -5.53 54.35 /
PLOG/ 0.01 6.70E+25 -6.13 59.16 /
PLOG/ 0.03 2.20E+27 -6.37 62.68 /
PLOG/ 0.1 8.70E+28 -6.60 66.99 /
PLOG/ 0.3 3.40E+29 -6.55 70.29 /
PLOG/ 1.0 2.70E+29 -6.27 73.35 /
PLOG/ 3.0 2.20E+28 -5.71 75.06 /
PLOG/ 10.0 1.50E+26 -4.82 75.60 /
PLOG/ 30.0 2.10E+23 -3.77 74.56 /
PLOG/ 100.0 4.40E+18 -2.17 70.46 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H4_Olef+HO2r=cC2H4O+HO_r

1.30E+07 1.54 59.08 ! 1 atm
PLOG/ 1.0E-4 1.00E+04 2.42 50.42 /
PLOG/ 3.0E-4 1.10E+04 2.41 50.46 /
PLOG/ 0.001 1.10E+04 2.41 50.50 /
PLOG/ 0.003 1.20E+04 2.41 50.54 /
PLOG/ 0.01 1.30E+04 2.39 50.71 /
PLOG/ 0.03 2.00E+04 2.34 51.17 /
PLOG/ 0.1 6.00E+04 2.20 52.43 /
PLOG/ 0.3 4.20E+05 1.96 54.77 /
PLOG/ 1.0 1.30E+07 1.54 59.08 /
PLOG/ 3.0 9.30E+08 1.02 64.73 /
PLOG/ 10.0 1.10E+11 0.45 72.05 /
PLOG/ 30.0 2.10E+12 0.11 78.45 /
PLOG/ 100.0 2.20E+12 0.16 83.60 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

C2H4_Olef+O2=C2H3r_Olef+HO2r

7.10E+13 0.00 251.08 !

! Hua H Ruscic B Wang B CP 311:335-341 2005

!

!C2H4_Olef+CH3r=C2H3r_Olef+CH4

9.80E+02 2.95 63.38 !

!DUP

! Miller and Klippenstein, J. Phys. Chem. A 2013, 117, 2718-2727

!

C2H4_Olef+CH2(S)=C2H3r_Olef+CH3r

4.20E+24 -3.19 40.83 ! 1 atm
PLOG/ 0.01 1.80E+19 -1.95 28.40 /
PLOG/ 0.1 1.70E+19 -1.80 18.03 /
PLOG/ 1.0 4.20E+24 -3.19 40.83 /
PLOG/ 10.0 7.90E+24 -3.08 58.13 /
PLOG/ 100.0 7.40E+29 -4.28 99.78 /

DUP

C2H4_Olef+CH2(S)=C2H3r_Olef+CH3r

4.90E+09 1.02 2.51 ! 1 atm
PLOG/ 0.01 4.30E+12 0.19 -0.46 /
PLOG/ 0.1 2.30E+11 0.54 0.20 /
PLOG/ 1.0 4.90E+09 1.02 2.51 /
PLOG/ 10.0 1.50E+08 1.33 5.14 /
PLOG/ 100.0 8.10E+10 0.55 23.04 /

DUP

! Ye, Georgievskii, Klippenstein, Proc. Combust. Inst. 35 (2015) 223-230
!

C2H2+Hr(+M)=C2H3r_Olef(+M)

1.70E+10 1.27 11.33 !
LOW/ 6.30E+31 -4.66 15.82 /
TROE/ 0.7878 -10212.0 1.0E-30 /
CO/ 2.0/ CO2/ 3.0/ H2/ 2.0/ H2O/ 5.0/

! Miller JA Klippenstein PCCP 6:1192-1202 2004

!

C2H3r_Olef+Hr=C2H2+H2

4.50E+13 0.00 0.00 !

! Monks PS Nesbitt FL Payne WA Scanlon M Stief LJ Shallcross DE JPC
99:17151-17159 1995

!

C2H3r_Olef+Or=CH2CO+Hr

3.00E+13 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

C2H3r_Olef+HOr=C2H2+H2O

2.00E+13 0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998

! JAM est

!

C2H3r_Olef+HO2r=CH2CHO+HOr

3.00E+13 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986

!

C2H3r_Olef+O2=CH2CHOO

3.30E+61 -15.79 84.31 ! 1 atm
PLOG/ 0.01 1.60E+24 -5.45 40.43 /
PLOG/ 0.1 3.50E+56 -15.01 80.17 /
PLOG/ 0.316 1.30E+64 -16.97 89.08 /
PLOG/ 1.0 3.30E+61 -15.79 84.31 /
PLOG/ 3.16 7.30E+53 -13.11 72.38 /
PLOG/ 10.0 4.20E+48 -11.21 66.94 /
PLOG/ 31.6 2.30E+43 -9.38 61.97 /
PLOG/ 100.0 3.40E+39 -8.04 60.08 /

DUP

C2H3r_Olef+O2=CH2CHOO

6.10E+28 -5.89 13.20 ! 1 atm
PLOG/ 0.01 1.80E-09 4.15 -19.69 /
PLOG/ 0.1 2.40E+22 -4.52 11.88 /

PLOG/ 0.316 2.00E+26 -5.43 11.40 /
PLOG/ 1.0 6.10E+28 -5.89 13.20 /
PLOG/ 3.16 2.10E+29 -5.80 14.73 /
PLOG/ 10.0 3.50E+28 -5.37 15.21 /
PLOG/ 31.6 3.30E+27 -4.95 15.10 /
PLOG/ 100.0 1.00E+27 -4.72 15.40 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CHCHO+HOr

2.80E+14 -1.83 0.02 ! 1 atm
PLOG/ 0.01 3.90E+11 -0.11 8.92 /
PLOG/ 0.1 1.10E+09 0.55 0.19 /
PLOG/ 0.316 8.50E+08 0.56 0.00 /
PLOG/ 1.0 2.80E+14 -1.83 0.02 /
PLOG/ 3.16 2.60E+20 -2.84 31.51 /
PLOG/ 10.0 9.20E+14 -2.26 0.00 /
PLOG/ 31.6 6.10E+25 -4.21 54.60 /
PLOG/ 100.0 1.70E+30 -5.35 77.11 /

DUP

C2H3r_Olef+O2=CHCHO+HOr

5.00E+11 -0.14 8.35 ! 1 atm
PLOG/ 0.01 9.90E+11 -0.66 -0.00 /
PLOG/ 0.1 6.90E+14 -1.16 19.00 /
PLOG/ 0.316 2.80E+13 -0.72 14.56 /
PLOG/ 1.0 5.00E+11 -0.14 8.35 /
PLOG/ 3.16 2.40E+10 0.23 6.58 /
PLOG/ 10.0 1.70E+14 -0.82 18.62 /
PLOG/ 31.6 1.40E+11 0.05 15.79 /
PLOG/ 100.0 3.20E+11 -0.02 22.33 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CH2CO+HOr

1.10E+03 2.39 25.86 ! 1 atm
PLOG/ 0.01 8.70E+02 2.41 25.36 /
PLOG/ 0.1 8.90E+02 2.41 25.43 /
PLOG/ 0.316 9.40E+02 2.40 25.57 /
PLOG/ 1.0 1.10E+03 2.39 25.86 /
PLOG/ 3.16 1.10E+03 2.38 25.85 /
PLOG/ 10.0 1.40E+03 2.36 25.41 /
PLOG/ 31.6 2.50E+06 1.42 35.48 /
PLOG/ 100.0 1.70E+10 0.36 50.25 /

DUP

C2H3r_Olef+O2=CH2CO+HOr

5.30E-01 3.01 7.43 ! 1 atm
PLOG/ 0.01 1.80E-01 3.12 5.57 /
PLOG/ 0.1 2.10E-01 3.11 5.79 /
PLOG/ 0.316 2.70E-01 3.08 6.26 /
PLOG/ 1.0 5.30E-01 3.01 7.43 /
PLOG/ 3.16 1.40E+00 2.90 9.31 /
PLOG/ 10.0 4.20E-01 2.93 8.59 /
PLOG/ 31.6 1.20E-04 4.21 8.55 /
PLOG/ 100.0 1.30E-03 3.97 14.28 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CH2CHO+Or

	6.50E+20	-2.65	27.15	!	1 atm
PLOG/	0.01	7.20E+20	-2.67	28.21	/
PLOG/	0.1	7.00E+20	-2.67	28.09	/
PLOG/	0.316	9.00E+20	-2.70	28.13	/
PLOG/	1.0	6.50E+20	-2.65	27.15	/
PLOG/	3.16	4.10E+20	-2.53	26.80	/
PLOG/	10.0	1.60E+23	-3.22	36.39	/
PLOG/	31.6	2.90E+25	-3.77	48.24	/
PLOG/	100.0	9.30E+25	-3.80	58.20	/

DUP

C2H3r_Olef+O2=CH2CHO+Or

	1.80E+10	0.58	0.16	!	1 atm
PLOG/	0.01	1.20E+10	0.62	-1.16	/
PLOG/	0.1	1.30E+10	0.62	-1.04	/
PLOG/	0.316	1.50E+10	0.60	-0.68	/
PLOG/	1.0	1.80E+10	0.58	0.16	/
PLOG/	3.16	8.90E+09	0.67	1.04	/
PLOG/	10.0	6.70E+09	0.72	3.26	/
PLOG/	31.6	1.40E+09	0.92	5.10	/
PLOG/	100.0	7.10E+07	1.28	5.86	/

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=C2H2+HO2r

	2.20E+07	1.19	14.09	!	1 atm
PLOG/	0.01	1.10E+07	1.28	13.90	/
PLOG/	0.1	7.80E+06	1.33	13.46	/
PLOG/	0.316	1.20E+07	1.27	13.85	/
PLOG/	1.0	2.20E+07	1.19	14.09	/
PLOG/	3.16	1.10E+08	1.00	15.46	/
PLOG/	10.0	1.30E+11	0.12	24.57	/
PLOG/	31.6	1.20E+09	0.82	23.50	/
PLOG/	100.0	1.10E+17	-1.45	51.17	/

DUP

C2H3r_Olef+O2=C2H2+HO2r

	4.60E+01	2.76	-2.06	!	1 atm
PLOG/	0.01	4.80E+01	2.75	-3.33	/
PLOG/	0.1	5.20E+01	2.73	-3.21	/
PLOG/	0.316	5.60E+01	2.73	-2.76	/
PLOG/	1.0	4.60E+01	2.76	-2.06	/
PLOG/	3.16	3.80E+00	3.07	-2.51	/
PLOG/	10.0	5.50E+00	3.07	0.36	/
PLOG/	31.6	4.50E+08	-0.00	4.00	/
PLOG/	100.0	2.00E+01	2.94	7.73	/

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=OCHCHO+Hr
3.70E+15 -1.29 6.03 ! 1 atm
PLOG/ 0.01 4.80E+14 -1.03 3.82 /
PLOG/ 0.1 5.00E+14 -1.04 3.86 /
PLOG/ 0.316 6.40E+14 -1.07 4.11 /
PLOG/ 1.0 3.70E+15 -1.29 6.03 /
PLOG/ 3.16 2.40E+18 -2.13 13.53 /
PLOG/ 10.0 1.30E+15 -1.09 10.01 /
PLOG/ 31.6 3.60E+33 -6.50 62.38 /
PLOG/ 100.0 3.30E+31 -5.76 67.99 /

DUP

C2H3r_Olef+O2=OCHCHO+Hr
5.00E-01 3.15 -23.00 ! 1 atm
PLOG/ 0.01 2.80E-04 4.04 -29.37 /
PLOG/ 0.1 3.50E-04 4.01 -29.20 /
PLOG/ 0.316 9.70E-04 3.89 -28.32 /
PLOG/ 1.0 5.00E-01 3.15 -23.00 /
PLOG/ 3.16 1.30E+05 1.67 -12.26 /
PLOG/ 10.0 4.50E+15 -3.08 -20.23 /
PLOG/ 31.6 3.80E+10 0.22 3.94 /
PLOG/ 100.0 2.80E+08 0.83 3.59 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

!C2H3r_Olef+O2=CH2O+HCO
3.00E+35 -7.32 49.45 ! 1 atm
! PLOG/ 0.01 1.40E+36 -7.60 52.76 /
! PLOG/ 0.1 2.60E+15 -1.28 2.15 /
! PLOG/ 0.316 2.20E+36 -7.57 52.26 /
! PLOG/ 1.0 3.00E+35 -7.32 49.45 /
! PLOG/ 3.16 1.60E+36 -7.47 52.13 /
! PLOG/ 10.0 5.80E+35 -7.20 56.19 /
! PLOG/ 31.6 3.50E+20 -2.57 23.34 /
! PLOG/ 100.0 3.00E+33 -6.28 66.94 /

!DUP

!C2H3r_Olef+O2=CH2O+HCO
6.80E+15 -1.31 2.70 ! 1 atm
! PLOG/ 0.01 1.40E+36 -7.60 52.76 /
! PLOG/ 0.1 2.50E+15 -1.28 2.15 /
! PLOG/ 0.316 5.30E+15 -1.29 2.18 /
! PLOG/ 1.0 6.80E+15 -1.31 2.70 /
! PLOG/ 3.16 1.10E+16 -1.36 4.46 /
! PLOG/ 10.0 2.80E+15 -1.18 5.98 /
! PLOG/ 31.6 1.10E+69 -19.23 61.76 /
! PLOG/ 100.0 4.70E+10 0.19 3.48 /

!DUP

C2H3r_Olef+O2=CH2O+HCO
1.700E+29 -5.312 27.2 !! AramcoMech

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CH2O+Hr+CO
7.10E+35 -7.32 49.45 ! 1 atm

PLOG/ 0.01 6.50E+36 -7.60 52.89 /
PLOG/ 0.1 6.30E+36 -7.60 52.76 /
PLOG/ 0.316 5.10E+36 -7.57 52.26 /
PLOG/ 1.0 7.10E+35 -7.32 49.45 /
PLOG/ 3.16 3.70E+36 -7.47 52.13 /
PLOG/ 10.0 1.30E+36 -7.20 56.19 /
PLOG/ 31.6 8.30E+20 -2.57 23.34 /
PLOG/ 100.0 7.10E+33 -6.28 66.94 /

DUP

C2H3r_Olef+O2=CH2O+Hr+CO

1.60E+16 -1.31 2.70 ! 1 atm
PLOG/ 0.01 1.20E+16 -1.28 2.15 /
PLOG/ 0.1 1.20E+16 -1.28 2.15 /
PLOG/ 0.316 1.30E+16 -1.29 2.18 /
PLOG/ 1.0 1.60E+16 -1.31 2.70 /
PLOG/ 3.16 2.40E+16 -1.36 4.46 /
PLOG/ 10.0 6.60E+15 -1.18 5.98 /
PLOG/ 31.6 2.70E+69 -19.23 61.76 /
PLOG/ 100.0 1.10E+11 0.19 3.48 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CO+CH3O

1.00E+11 -0.33 -3.13 ! 1 atm
PLOG/ 0.01 8.20E+18 -2.66 13.39 /
PLOG/ 0.1 4.10E+14 -1.32 3.71 /
PLOG/ 0.316 4.30E+14 -1.33 3.77 /
PLOG/ 1.0 1.00E+11 -0.33 -3.13 /
PLOG/ 3.16 1.90E+12 -3.00 -37.64 /
PLOG/ 10.0 1.90E+24 -5.63 0.01 /
PLOG/ 31.6 1.10E+18 -2.22 21.66 /
PLOG/ 100.0 5.80E+32 -6.45 70.33 /

DUP

C2H3r_Olef+O2=CO+CH3O

5.80E+21 -3.54 19.97 ! 1 atm
PLOG/ 0.01 1.30E+09 0.18 -7.18 /
PLOG/ 0.1 6.00E+11 -2.93 -40.02 /
PLOG/ 0.316 2.90E+11 -2.93 -42.34 /
PLOG/ 1.0 5.80E+21 -3.54 19.97 /
PLOG/ 3.16 5.00E+15 -1.62 7.74 /
PLOG/ 10.0 9.30E+16 -1.96 13.91 /
PLOG/ 31.6 1.00E+72 -20.69 66.36 /
PLOG/ 100.0 1.10E+09 0.31 4.28 /

DUP

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

!

C2H3r_Olef+O2=CO2+CH3r

7.30E+31 -6.70 43.68 ! 1 atm
PLOG/ 0.01 2.40E+35 -7.76 52.84 /
PLOG/ 0.1 1.70E+35 -7.72 52.38 /
PLOG/ 0.316 4.50E+34 -7.55 50.79 /
PLOG/ 1.0 7.30E+31 -6.70 43.68 /
PLOG/ 3.16 3.60E+35 -7.75 53.68 /
PLOG/ 10.0 2.10E+35 -7.53 58.79 /

```

PLOG/ 31.6 3.80E+18 -2.44 22.63 /
PLOG/ 100.0 1.20E+32 -6.32 67.74 /
DUP
C2H3r_Olef+O2=CO2+CH3r
5.30E+13 -1.14 1.87 ! 1 atm
PLOG/ 0.01 6.30E+13 -1.16 1.70 /
PLOG/ 0.1 6.20E+13 -1.16 1.68 /
PLOG/ 0.316 6.10E+13 -1.16 1.66 /
PLOG/ 1.0 5.30E+13 -1.14 1.87 /
PLOG/ 3.16 1.50E+14 -1.26 4.13 /
PLOG/ 10.0 5.00E+13 -1.11 5.90 /
PLOG/ 31.6 1.40E+70 -20.11 64.56 /
PLOG/ 100.0 9.20E+08 0.25 3.58 /
DUP
! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J.
Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).
!
C2H3r_Olef+CH2O=C2H4_Olef+HCO
1.40E+10 0.21 16.46 ! 1 atm
PLOG/ 0.001 1.10E+07 1.09 7.56 /
PLOG/ 0.01 2.50E+07 0.99 8.35 /
PLOG/ 0.1 2.50E+08 0.70 10.86 /
PLOG/ 1.0 1.40E+10 0.21 16.46 /
PLOG/ 10.0 3.50E+13 -0.73 29.05 /
PLOG/ 100.0 3.30E+14 -0.87 45.88 /
PLOG/ 1000.0 1.70E+01 3.17 39.33 /
DUP
C2H3r_Olef+CH2O=C2H4_Olef+HCO
-8.50E19 -2.26 99.84 ! 1 atm
PLOG/ 0.001 -2.30E16 -1.27 86.26 /
PLOG/ 0.01 -5.20E16 -1.37 87.05 /
PLOG/ 0.1 -1.50E18 -1.77 94.24 /
PLOG/ 1.0 -8.50E19 -2.26 99.84 /
PLOG/ 10.0 -4.40E23 -3.28 116.29 /
PLOG/ 100.0 -4.20E24 -3.42 133.12 /
PLOG/ 1000.0 -2.10E11 0.62 126.57 /
DUP
! C.F. Goldsmith et al., J. Phys. Chem. A 116 (2012) 3325-3346.
!
C2H3r_Olef+CH2O=C2H4_Olef+Hr+CO
8.50E+19 -2.26 99.84 ! 1 atm
PLOG/ 0.001 2.30E+16 -1.27 86.26 /
PLOG/ 0.01 5.20E+16 -1.37 87.05 /
PLOG/ 0.1 1.50E+18 -1.77 94.24 /
PLOG/ 1.0 8.50E+19 -2.26 99.84 /
PLOG/ 10.0 4.40E+23 -3.28 116.29 /
PLOG/ 100.0 4.20E+24 -3.42 133.12 /
PLOG/ 1000.0 2.10E+11 0.62 126.57 /
!
C2H3r_Olef+HCO=C2H4_Olef+CO
9.00E+13 0.00 0.00 !
! Tsang W Hampson RF JPCRD 15:1087 1986
!
```

```

!!C2H3r_Olef+CH3r=C2H2+CH4
      9.00E+12    0.00 -3.20 !

! Stoliarov SI Knyazev VD Slagle IR JPCA 104:9687-9697 2000
!
C2H3r_Olef+CH=CH2+C2H2
      5.00E+13    0.00 0.00 !

! JAM est
!
C2H3r_Olef+CH3OH=C2H4_Olef+CH3O
      1.00E+06    1.51 111.42    !

! Chen et al., Int. J. Chem. Kinet. 47 (2015) 764-772
!
C2H3r_Olef+CH3OH=C2H4_Olef+CH2OH
1.80E-02    4.02 97.78 !

! Chen et al., Int. J. Chem. Kinet. 47 (2015) 764--772
!
C2H3r_Olef+C2H3r_Olef=C2H4_Olef+C2H2
1.50E+13    0.00 0.00 !

! Fahr A Laufer A Klein R Braun W JPC 95:3218-3224 1991
!
C2H3r_Olef+C2H=C2H2+C2H2
      3.00E+13    0.00 0.00 !

! JAM est
!
C2H2+M=C2H+Hr+M
      9.10E+30   -3.70 531.95    !
CO/   2.0/ CO2/ 3.0/ H2/   2.0/ H2O/ 5.0/

! Tsang W Hampson RF JPCRD 15:1087 1986
!
C2H2 (+M)=H2CC (+M)
      1.80E+04    3.51 181.17    !
LOW/   2.50E+15   -0.64 207.94    /
TROE/ 0.5   1.0E-30    1.0E30    /

! pw
!
C2H+H2=C2H2+Hr
      4.10E+05    2.39 3.61    !

! Harding LB Schatz GC Chiles RA JCP 76:5172-5173 1982
!
C2H2+Or=HCCO+Hr
      1.40E+07    2.00 7.95    !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
!
C2H2+Or=CH2+CO
      6.10E+06    2.00 7.95    !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
!

```

!C2H2+O=C2H+OH 3.2E15 -0.600 15000 ! # reverse
too fast with present thermochemistry
! P Glarborg RJ Kee JA Miller CNF 65 (1986) 177-202.
!

C2H2+HOr=CH3r+CO

1.30E+09 0.73 10.79 ! 1 atm
PLOG/ 0.01 4.80E+05 1.68 -1.38 /
PLOG/ 0.025 4.40E+06 1.40 0.95 /
PLOG/ 0.1 7.70E+07 1.05 4.67 /
PLOG/ 1.0 1.30E+09 0.73 10.79 /
PLOG/ 10.0 4.30E+08 0.92 15.63 /
PLOG/ 100.0 8.30E+05 1.77 19.65 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005
!

C2H2+HOr=HCCOH+Hr

2.40E+06 2.00 53.19 ! 1 atm
PLOG/ 0.01 2.80E+05 2.28 51.96 /
PLOG/ 0.025 7.50E+05 2.16 52.50 /
PLOG/ 0.1 1.80E+06 2.04 53.01 /
PLOG/ 1.0 2.40E+06 2.00 53.19 /
PLOG/ 10.0 3.20E+06 1.97 53.60 /
PLOG/ 100.0 7.40E+06 1.89 56.91 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005
!

C2H2+HOr=CHCHOH

1.90E+44 -11.38 26.36 ! 1 atm
PLOG/ 0.01 2.90E+64 -18.57 41.88 /
PLOG/ 0.025 4.70E+59 -16.87 38.02 /
PLOG/ 0.1 1.20E+28 -5.56 15.58 /
PLOG/ 1.0 1.90E+44 -11.38 26.36 /
PLOG/ 10.0 1.50E+24 -4.06 13.64 /
PLOG/ 100.0 6.20E+20 -2.80 11.84 /

DUP

C2H2+HOr=CHCHOH

3.50E+31 -6.20 27.76 ! 1 atm
PLOG/ 0.01 2.60E+33 -7.36 26.74 /
PLOG/ 0.025 4.40E+32 -7.02 24.82 /
PLOG/ 0.1 6.40E+42 -9.96 49.11 /
PLOG/ 1.0 3.50E+31 -6.20 27.76 /
PLOG/ 10.0 4.50E+31 -5.92 36.66 /
PLOG/ 100.0 1.60E+29 -4.91 40.73 /

DUP

! Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005
!

C2H2+HOr=CH2CO+Hr

7.50E+06 1.55 8.81 ! 1 atm
PLOG/ 0.01 1.70E+03 2.56 -3.53 /
PLOG/ 0.025 1.50E+04 2.28 -1.22 /
PLOG/ 0.1 3.00E+05 1.92 2.50 /
PLOG/ 1.0 7.50E+06 1.55 8.81 /
PLOG/ 10.0 5.10E+06 1.65 14.23 /
PLOG/ 100.0 1.50E+04 2.45 18.73 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005
!

C2H2+HOr=C2H+H2O
2.60E+06 2.14 71.38 !

!Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005
!

C2H2+HO2r=CH2CHOO
4.10E+50 -13.07 113.89 ! 1 atm
PLOG/ 0.01 5.00E+06 -1.02 38.29 /
PLOG/ 0.1 6.00E+17 -3.82 45.15 /
PLOG/ 0.316 2.50E+48 -12.82 105.52 /
PLOG/ 1.0 4.10E+50 -13.07 113.89 /
PLOG/ 3.16 9.10E+46 -11.57 112.47 /
PLOG/ 10.0 4.60E+43 -10.24 112.68 /
PLOG/ 31.6 5.60E+38 -8.49 109.66 /
PLOG/ 100.0 2.50E+35 -7.26 110.42 /

DUP

C2H2+HO2r=CH2CHOO
4.90E+21 -4.37 51.13 ! 1 atm
PLOG/ 0.01 1.90E+26 -8.34 38.70 /
PLOG/ 0.1 5.30E+129 -41.74 150.33 /
PLOG/ 0.316 2.00E+18 -3.67 43.85 /
PLOG/ 1.0 4.90E+21 -4.37 51.13 /
PLOG/ 3.16 1.90E+22 -4.28 54.73 /
PLOG/ 10.0 2.10E+21 -3.78 55.98 /
PLOG/ 31.6 1.40E+20 -3.30 56.11 /
PLOG/ 100.0 1.40E+19 -2.91 56.15 /

DUP

C2H2+HO2r=CHCHO+HOr
1.60E+10 0.77 79.66 ! 1 atm
PLOG/ 0.01 5.50E+09 0.91 77.40 /
PLOG/ 0.1 5.90E+09 0.90 77.61 /
PLOG/ 0.316 6.80E+09 0.88 77.99 /
PLOG/ 1.0 1.60E+10 0.77 79.66 /
PLOG/ 3.16 3.50E+09 0.99 78.70 /
PLOG/ 10.0 5.40E+10 0.61 86.78 /
PLOG/ 31.6 3.70E+08 1.23 66.78 /
PLOG/ 100.0 1.50E+11 0.48 74.18 /

DUP

C2H2+HO2r=CHCHO+HOr
2.50E+07 1.56 61.88 ! 1 atm
PLOG/ 0.01 2.40E+07 1.54 61.46 /
PLOG/ 0.1 2.50E+07 1.54 61.50 /
PLOG/ 0.316 2.60E+07 1.54 61.63 /
PLOG/ 1.0 2.50E+07 1.56 61.88 /
PLOG/ 3.16 1.50E+08 1.32 63.14 /
PLOG/ 10.0 1.60E+08 1.36 64.52 /
PLOG/ 31.6 1.70E+07 1.59 66.57 /
PLOG/ 100.0 7.20E+06 1.73 67.03 /

DUP

C2H2+HO2r=CH2CO+HOr
5.30E-07 4.78 64.68 ! 1 atm
PLOG/ 0.01 6.30E-07 4.75 64.98 /
PLOG/ 0.1 6.70E-07 4.74 65.06 /
PLOG/ 0.316 4.20E-07 4.81 64.48 /
PLOG/ 1.0 5.30E-07 4.78 64.68 /
PLOG/ 3.16 1.00E-06 4.69 65.44 /
PLOG/ 10.0 4.70E-05 4.22 70.21 /
PLOG/ 31.6 9.00E-01 2.97 82.55 /

PLOG/ 100.0 3.60E+03 1.97 96.27 /

DUP

C2H2+HO2r=CH2CO+HOr

3.30E-15 6.70 42.22 ! 1 atm

PLOG/ 0.01 1.30E-14 6.58 42.97 /

PLOG/ 0.1 1.30E-14 6.59 43.22 /

PLOG/ 0.316 4.00E-14 6.36 42.97 /

PLOG/ 1.0 3.30E-15 6.70 42.22 /

PLOG/ 3.16 8.70E-21 8.30 33.92 /

PLOG/ 10.0 8.40E-22 8.76 36.84 /

PLOG/ 31.6 6.90E-14 6.67 54.94 /

PLOG/ 100.0 6.60E-12 6.15 61.63 /

DUP

C2H2+HO2r=CH2CHO+Or

3.00E+07 0.98 55.69 ! 1 atm

PLOG/ 0.01 5.50E+00 1.19 53.89 /

PLOG/ 0.1 1.10E+08 0.77 56.90 /

PLOG/ 0.316 1.20E+07 1.09 54.60 /

PLOG/ 1.0 3.00E+07 0.98 55.69 /

PLOG/ 3.16 2.00E+74 -16.33 456.89 /

PLOG/ 10.0 7.50E+14 -1.17 76.78 /

PLOG/ 31.6 8.60E+18 -2.27 93.01 /

PLOG/ 100.0 5.80E+18 -2.09 101.88 /

DUP

C2H2+HO2r=CH2CHO+Or

2.50E-04 4.19 34.32 ! 1 atm

PLOG/ 0.01 2.90E-04 4.16 32.37 /

PLOG/ 0.1 6.10E+03 3.81 35.12 /

PLOG/ 0.316 5.40E-04 4.09 33.66 /

PLOG/ 1.0 2.50E-04 4.19 34.32 /

PLOG/ 3.16 6.60E+04 1.85 51.71 /

PLOG/ 10.0 2.90E-01 3.38 44.31 /

PLOG/ 31.6 2.00E+00 3.17 49.12 /

PLOG/ 100.0 1.10E-01 3.52 50.12 /

DUP

C2H2+HO2r=OCHCHO+Hr

2.20E+09 0.06 52.17 ! 1 atm

PLOG/ 0.01 8.50E+07 0.48 49.04 /

PLOG/ 0.1 7.40E+07 0.50 48.91 /

PLOG/ 0.316 7.90E+07 0.49 48.95 /

PLOG/ 1.0 2.20E+09 0.06 52.17 /

PLOG/ 3.16 7.00E+49 -10.18 322.63 /

PLOG/ 10.0 4.10E+16 -2.03 73.76 /

PLOG/ 31.6 9.40E+16 -2.03 81.96 /

PLOG/ 100.0 5.90E+21 -3.32 104.73 /

DUP

C2H2+HO2r=OCHCHO+Hr

2.20E-05 4.17 26.84 ! 1 atm

PLOG/ 0.01 2.40E-06 4.43 23.34 /

PLOG/ 0.1 2.00E-06 4.45 23.28 /

PLOG/ 0.316 1.80E-06 4.46 23.66 /

PLOG/ 1.0 2.20E-05 4.17 26.84 /

PLOG/ 3.16 7.70E+05 1.18 47.45 /

PLOG/ 10.0 2.00E-02 3.38 36.38 /

PLOG/ 31.6 6.10E-03 3.53 38.56 /

PLOG/ 100.0 6.80E-02 3.27 45.02 /

DUP

! Replace HCO with 70% H + CO

C2H2+HO2r=CH2O+HCO

	3.30E+102	-24.18	579.90	! 1 atm
PLOG/ 0.01	3.90E+13	-1.17	57.53	/
PLOG/ 0.1	4.30E+00	2.64	30.35	/
PLOG/ 0.316	2.60E-06	4.34	18.93	/
PLOG/ 1.0	3.30E+102	-24.18	579.90	/
PLOG/ 3.16	5.20E+15	-1.75	63.51	/
PLOG/ 10.0	7.30E+35	-7.77	112.84	/
PLOG/ 31.6	1.80E+28	-5.30	105.14	/
PLOG/ 100.0	2.50E+16	-1.70	83.81	/

DUP

C2H2+HO2r=CH2O+HCO

	8.10E+07	0.60	45.40	! 1 atm
PLOG/ 0.01	8.40E+00	2.56	30.89	/
PLOG/ 0.1	1.60E+13	-1.05	56.57	/
PLOG/ 0.316	6.90E+09	-0.00	49.04	/
PLOG/ 1.0	8.10E+07	0.60	45.40	/
PLOG/ 3.16	3.50E+00	2.69	33.58	/
PLOG/ 10.0	9.80E+06	0.91	48.99	/
PLOG/ 31.6	1.80E+04	1.70	47.07	/
PLOG/ 100.0	4.30E-06	4.31	28.57	/

DUP

C2H2+HO2r=CH2O+Hr+CO

	7.80E+102	-24.18	579.90	! 1 atm
PLOG/ 0.01	9.10E+13	-1.17	57.53	/
PLOG/ 0.1	9.90E+00	2.64	30.35	/
PLOG/ 0.316	6.10E-06	4.34	18.93	/
PLOG/ 1.0	7.80E+102	-24.18	579.90	/
PLOG/ 3.16	1.20E+16	-1.75	63.51	/
PLOG/ 10.0	1.70E+36	-7.77	112.84	/
PLOG/ 31.6	4.10E+28	-5.30	105.14	/
PLOG/ 100.0	5.80E+16	-1.70	83.81	/

DUP

C2H2+HO2r=CH2O+Hr+CO

	1.90E+08	0.60	45.40	! 1 atm
PLOG/ 0.01	2.00E+01	2.56	30.89	/
PLOG/ 0.1	3.60E+13	-1.05	56.57	/
PLOG/ 0.316	1.60E+10	-0.00	49.04	/
PLOG/ 1.0	1.90E+08	0.60	45.40	/
PLOG/ 3.16	8.30E+00	2.69	33.58	/
PLOG/ 10.0	2.30E+07	0.91	48.99	/
PLOG/ 31.6	4.20E+04	1.70	47.07	/
PLOG/ 100.0	1.00E-05	4.31	28.57	/

DUP

C2H2+HO2r=CO+CH3O

	8.90E+69	-15.85	428.86	! 1 atm
PLOG/ 0.01	3.50E+11	0.00	207.15	/
PLOG/ 0.1	2.80E+08	0.01	49.87	/
PLOG/ 0.316	8.10E+07	0.18	48.74	/
PLOG/ 1.0	8.90E+69	-15.85	428.86	/
PLOG/ 3.16	5.70E+12	-1.25	60.96	/
PLOG/ 10.0	3.30E+23	-4.45	88.74	/
PLOG/ 31.6	2.40E+22	-3.96	94.77	/
PLOG/ 100.0	1.20E+18	-2.57	93.55	/

DUP

C2H2+HO2r=CO+CH3O

	5.40E+05	0.86	44.77	! 1 atm
--	----------	------	-------	---------

```

PLOG/ 0.01 2.90E+04 1.23 41.43 /
PLOG/ 0.1 9.70E-07 4.15 21.64 /
PLOG/ 0.316 1.80E-08 4.62 18.90 /
PLOG/ 1.0 5.40E+05 0.86 44.77 /
PLOG/ 3.16 5.40E-04 3.42 30.20 /
PLOG/ 10.0 2.90E+02 1.84 43.76 /
PLOG/ 31.6 8.10E+00 2.30 44.18 /
PLOG/ 100.0 6.90E-04 3.42 39.03 /

DUP
C2H2+HO2r=CO2+CH3r
      4.00E+84 -19.80 501.24 ! 1 atm
PLOG/ 0.01 1.20E-07 4.31 19.30 /
PLOG/ 0.1 1.10E-07 4.32 19.34 /
PLOG/ 0.316 1.80E+142 -35.04 789.52 /
PLOG/ 1.0 4.00E+84 -19.80 501.24 /
PLOG/ 3.16 5.00E+13 -1.60 62.68 /
PLOG/ 10.0 8.60E+28 -6.15 100.54 /
PLOG/ 31.6 1.30E+27 -5.42 106.19 /
PLOG/ 100.0 1.70E+15 -1.80 85.23 /

DUP
C2H2+HO2r=CO2+CH3r
      1.40E+06 0.68 45.23 ! 1 atm
PLOG/ 0.01 2.00E+08 0.00 49.33 /
PLOG/ 0.1 2.00E+08 0.00 49.29 /
PLOG/ 0.316 1.60E+05 0.95 42.68 /
PLOG/ 1.0 1.40E+06 0.68 45.23 /
PLOG/ 3.16 9.30E-03 3.00 32.05 /
PLOG/ 10.0 1.90E+04 1.26 46.99 /
PLOG/ 31.6 2.90E+02 1.79 47.03 /
PLOG/ 100.0 3.90E-07 4.21 30.60 /

DUP

! pw CFG 2015
!
C2H2+O2=HCO+HCO
      6.10E+12 0.00 222.80

DUP
C2H2+O2=HCO+HCO
      1.70E+07 1.67 296.90 ! triplet surface

DUP
C2H2+O2=HCO+Hr+CO
      6.70E+33 -5.63 344.49

DUP
C2H2+O2=HCO+Hr+CO
      1.10E+26 -3.52 309.44

DUP
C2H2+O2=Hr+CO+Hr+CO
      1.20E+32 -4.87 389.15 !

! Gimenez-Lopez et al. 2016 c2h2 paper
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
! Chem. Lett. 2016)
!
C2H2+CH2(S)=C2H2+CH2
      4.00E+13 0.00 0.00 !

! Hack W Koch M Wagener R Wagner HGg BBPC 93:165 1989
!
```

$H_2CC+Hr=C_2H_2+Hr$
 1.00E+14 0.00 0.00 !
 ! Laskin A Wang H Law CK IJCK 32:589 2000
 !
 $H_2CC+HOr=CH_2CO+Hr$
 2.00E+13 0.00 0.00 !
 ! Laskin A Wang H Law CK IJCK 32:589 2000
 !
 $H_2CC+O_2=CH_2+CO_2$
 1.00E+13 0.00 0.00 !
 ! Laskin A Wang H CPL 303:43-49 1999
 ! JAM est prod
 !
 $C_2+H_2=C_2H+Hr$
 4.00E+05 2.40 4.18 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 !
 $C_2H+Or=CH+CO$
 5.00E+13 0.00 0.00 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !
 $C_2H+HOr=HCCO+Hr$
 2.00E+13 0.00 0.00 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !
 $C_2H+HOr=C_2+H_2O$
 4.00E+07 2.00 33.47 !
 ! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
 ! JAM est
 !
 $C_2H+O_2=CO+CO+Hr$
 4.70E+13 -0.16 0.00 !
 ! Thiesemann H Taatjes CA CPL 270:580-586 1997
 !
 $C_2H+CH_4=CH_3r+C_2H_2$
 7.20E+12 0.00 4.08 !
 ! Opansky BJ Leone SR JPC 100:4888-4892 1996
 !
 $C_2+M=C+C+M$
 1.50E+16 0.00 595.38 !
 ! Kruse T Roth P JPCA 101:2138-2146 1997
 !
 $C_2+Or=C+CO$
 1.00E+14 0.00 0.00 !
 ! est

```

!
C2+HOr=C2O+Hr
      5.00E+13    0.00 0.00  !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
! JAM est
!
C2+O2=CO+CO
      9.00E+12    0.00 4.10  !

! Baughum SL Oldenberg RC ACS SS (ed TM Sloane) 249:257-266 1984
! JAM est prod
!
CH3CH2OH=CH2OH+CH3r
      5.60E+64   -14.47    447.85    ! 1 atm
PLOG/ 0.001  1.30E+51   -10.59    422.04    /
PLOG/ 0.01   5.20E+59   -13.98    417.77    /
PLOG/ 0.1    1.60E+66   -15.30    440.70    /
PLOG/ 1.0    5.60E+64   -14.47    447.85    /
PLOG/ 10.0   1.60E+58   -12.29    442.28    /
PLOG/ 100.0  1.80E+47   -8.96 422.59    /

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.
!
CH3CH2OH=C2H5r+HOr
      1.50E+65   -14.89    469.79    ! 1 atm
PLOG/ 0.001  8.10E+46   -11.33    464.39    /
PLOG/ 0.01   1.80E+56   -13.49    448.43    /
PLOG/ 0.1    4.70E+63   -14.99    458.40    /
PLOG/ 1.0    1.50E+65   -14.89    469.79    /
PLOG/ 10.0   2.80E+61   -13.40    472.86    /
PLOG/ 100.0  6.20E+51   -10.34    459.73    /

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.
!
CH3CH2OH=C2H4_Olef+H2O
      5.20E+43   -8.90 340.83    ! 1 atm
PLOG/ 0.001  3.40E+59   -14.22    349.89    /
PLOG/ 0.01   2.60E+57   -13.29    356.54    /
PLOG/ 0.1    1.70E+52   -11.52    354.38    /
PLOG/ 1.0    5.20E+43   -8.90 340.83    /
PLOG/ 10.0   4.60E+32   -5.60 318.06    /
PLOG/ 100.0  3.80E+20   -2.06 290.48    /

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.
!
CH3CHOH+Hr=CH3CH2OH
      1.20E+53   -12.33    60.69 ! 1 atm
PLOG/ 0.01   9.90E+42   -10.77    37.41 /
PLOG/ 0.1    1.90E+55   -13.56    59.86 /
PLOG/ 1.0    1.20E+53   -12.33    60.69 /
PLOG/ 10.0   1.70E+50   -11.04    66.51 /
PLOG/ 100.0  1.60E+40   -7.82 54.04 /

```

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455; personal communication 650-2000 K fit

!
!CH3CH2O+H(+M)=CH3CH2OH(+M) 3.1E11 0.894 13 !
! LOW / 3.8E51 -15.550 11101 /
! Xu et al., J. Phys. Chem. A 115 (2011) 3509-3522.
!

CH3CH2OH+Hr=CH3CHOH+H2
8.80E+03 2.68 12.19 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!
CH3CH2OH+Hr=CH2CH2OH+H2
5.30E+03 2.81 31.34 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!
CH3CH2OH+Hr=CH3CH2O+H2
9.50E+02 3.14 36.38 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding,
B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!
CH3CH2OH+Or=CH2CH2OH+HOr
9.70E+02 3.23 19.50 !

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

!
CH3CH2OH+Or=CH3CHOH+HOr
1.50E+05 2.47 3.67 !

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

!
CH3CH2OH+Or=CH3CH2O+HOr
1.50E-03 4.70 7.24 !

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

!
CH3CH2OH+HOr=CH3CHOH+H2O
4.50E+02 3.11 -11.15 !

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012)
59-88.

!
CH3CH2OH+HOr=CH2CH2OH+H2O
9.40E+03 2.67 -4.20 !

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012)
59-88.

!
CH3CH2OH+HOr=CH3CH2O+H2O
2.40E+03 2.82 -2.89 !

DUP
CH3CH2OH+HOr=CH3CH2O+H2O
7.90E+07 1.18 -1.27 !

DUP

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012) 59-88.

!
CH3CH2OH+HO2r=CH3CHOH+H2O2
8.20E+03 2.55 44.98 !

! Marinov NM IJCK 31:183 1999
!
CH3CH2OH+HO2r=CH2CH2OH+H2O2
1.20E+04 2.55 65.90 !

! Marinov NM IJCK 31:183 1999
!
CH3CH2OH+HO2r=CH3CH2O+H2O2
2.50E+12 0.00 100.42 !

! Marinov NM IJCK 31:183 1999
!
CH3CH2OH+CH3r=CH3CHOH+CH4
2.00E+01 3.37 31.92 !

! Xu et al., J. Chem. Phys. 120 (2004).
!
CH3CH2OH+CH3r=CH2CH2OH+CH4
2.00E+00 3.57 32.29 !

! Xu et al., J. Chem. Phys. 120 (2004).
!
CH3CH2OH+CH3r=CH3CH2O+CH4
3.30E+02 3.30 51.39 !

! Xu et al., J. Chem. Phys. 120 (2004).
!
CH3CHOH(+M)=CH3CHO+Hr(+M)
6.20E+09 1.31 141.33 !
LOW/ 1.80E+16 0.00 86.95 /
TROE/ 0.187 65.2 2568.0 41226.0 /

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176-188.
!
CH3CHOH(+M)=CH2CHOH+Hr(+M)
6.40E+09 1.33 150.52 !
LOW/ 8.20E+14 0.00 90.03 /
TROE/ 0.473 10.0 2218.0 2615.0 /

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176-188.
!
CH3CHOH(+M)=CH3r+CH2O(+M)
2.20E+09 1.18 142.20 !
LOW/ 5.90E+15 0.00 89.26 /
TROE/ 0.124 1.0 1729.0 50000.0 /

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176-188.
!
CH3CHOH+Hr=CH2CHOH+H2
3.10E+12 0.27 -1.40 !

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

CH3CHOH+Hr=C2H4_Olef+H2O

2.60E+20 -2.08 13.17 ! 1 atm
PLOG/ 0.001 1.20E+17 -1.17 1.19 /
PLOG/ 0.01 1.20E+17 -1.16 1.11 /
PLOG/ 0.1 1.80E+17 -1.22 1.62 /
PLOG/ 1.0 2.60E+20 -2.08 13.17 /
PLOG/ 10.0 9.30E+23 -3.00 33.28 /
PLOG/ 100.0 1.60E+20 -1.81 39.53 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

CH3CHOH+Hr=CH3r+CH2OH

2.30E+20 -1.79 24.66 ! 1 atm
PLOG/ 0.001 1.40E+17 -0.91 12.89 /
PLOG/ 0.01 1.50E+17 -0.92 13.04 /
PLOG/ 0.1 4.50E+17 -1.05 14.68 /
PLOG/ 1.0 2.30E+20 -1.79 24.66 /
PLOG/ 10.0 5.00E+24 -2.95 44.99 /
PLOG/ 100.0 4.00E+23 -2.53 57.06 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

CH3CHOH+Hr=C2H5r+HOr

1.60E+16 -0.70 27.94 ! 1 atm
PLOG/ 0.001 4.00E+13 0.02 18.59 /
PLOG/ 0.01 4.40E+13 0.01 18.73 /
PLOG/ 0.1 1.10E+14 -0.10 20.04 /
PLOG/ 1.0 1.60E+16 -0.70 27.94 /
PLOG/ 10.0 6.80E+20 -1.94 47.41 /
PLOG/ 100.0 6.30E+21 -2.11 63.89 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

CH3CHOH+Or=CH3CHO+HOr

1.00E+14 0.00 0.00 !

! Marinov NM IJCK 31:183 1999

!

CH3CHOH+HOr=CH3CHO+H2O

5.00E+12 0.00 0.00 !

! Marinov NM IJCK 31:183 1999

!

CH3CHOH+HO2r=CH3CHO+HOr+HOr

4.00E+13 0.00 0.00 !

! Marinov NM IJCK 31:183 1999

!

CH3CHOH+O2=CH3CHO+HO2r

5.30E+17 -1.64 3.51 ! 1 atm
PLOG/ 0.001 5.30E+17 -1.64 3.51 /
PLOG/ 0.01 5.30E+17 -1.64 3.51 /

PLOG/ 0.1 5.30E+17 -1.64 3.51 /
PLOG/ 1.0 5.30E+17 -1.64 3.51 /
PLOG/ 10.0 1.50E+18 -1.77 4.69 /
PLOG/ 100.0 3.80E+20 -2.43 12.93 /

! da Silva et al., J. Phys. Chem. A 113 (2009) 8923-8933

!

CH3CHOH+O2=CH2CHOH+HO2r

7.60E+02 2.45 -1.24 ! 1 atm
PLOG/ 0.001 5.10E+02 2.50 -1.73 /
PLOG/ 0.01 5.10E+02 2.50 -1.73 /
PLOG/ 0.1 5.30E+02 2.49 -1.68 /
PLOG/ 1.0 7.60E+02 2.45 -1.24 /
PLOG/ 10.0 8.90E+03 2.15 1.97 /
PLOG/ 100.0 4.40E+05 1.70 9.75 /

! da Silva et al., J. Phys. Chem. A 113 (2009) 8923-8933

!

CH2CH2OH=CH2CHOH+Hr

3.30E+28 -5.26 148.88 ! 1 atm
PLOG/ 0.0013 2.70E+15 -1.92 122.94 /
PLOG/ 1.0 3.30E+28 -5.26 148.88 /
PLOG/ 100.0 2.70E+27 -4.44 155.67 /

! Xu, Z. F.; Xu, K.; Lin, M. C. ChemPhysChem 2009, 10, 972-982

!CH3CH2O=CH2CH2OH 2.8E-29 11.900 4450 !

! Y. Zhang, S. Zhang, Q.S. Li, Chem. Phys. 308 (2005) 109-116 (kinf).

!

CH2CH2OH+Hr=C2H4_Olef+H2O

2.60E+22 -2.60 21.90 ! 1 atm
PLOG/ 0.001 1.70E+17 -1.18 1.40 /
PLOG/ 0.01 1.60E+17 -1.18 1.25 /
PLOG/ 0.1 1.70E+18 -1.46 4.63 /
PLOG/ 1.0 2.60E+22 -2.60 21.90 /
PLOG/ 10.0 6.50E+23 -2.88 38.94 /
PLOG/ 100.0 3.60E+16 -0.72 36.68 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!

CH2CH2OH+Hr=CH3r+CH2OH

1.90E+22 -2.30 32.19 ! 1 atm
PLOG/ 0.001 1.50E+17 -0.90 12.65 /
PLOG/ 0.01 1.90E+17 -0.94 13.05 /
PLOG/ 0.1 2.50E+18 -1.24 17.00 /
PLOG/ 1.0 1.90E+22 -2.30 32.19 /
PLOG/ 10.0 2.80E+25 -3.10 52.11 /
PLOG/ 100.0 7.50E+20 -1.69 56.19 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!

CH2CH2OH+Hr=C2H5r+HOr

9.20E+17 -1.16 34.28 ! 1 atm
PLOG/ 0.001 3.60E+13 0.05 18.00 /
PLOG/ 0.01 4.60E+13 0.02 18.38 /
PLOG/ 0.1 3.40E+14 -0.22 21.39 /
PLOG/ 1.0 9.20E+17 -1.16 34.28 /

PLOG/ 10.0 1.60E+22 -2.27 55.48 /
PLOG/ 100.0 8.10E+19 -1.51 64.99 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35
(2015) 447-455

!

CH2CH2OH+Hr(+M)=CH3CH2OH(+M)

5.20E+17 -0.99 6.61 !

LOW/ 2.00E+41 -7.08 27.97 /

TROE/ 0.8422 125.0 2219.0 6882.0 /

! est c2h5+h+m

!

CH2CH2OH+Or=CH2O+CH2OH

4.00E+13 0.00 0.00 !

! est C2H5+O

!

CH2CH2OH+HOr=CH2CHOH+H2O

7.90E+22 -2.99 16.16 ! 1 atm

PLOG/ 0.001 1.30E+19 -1.96 1.14 /

PLOG/ 0.01 1.20E+19 -1.95 1.00 /

PLOG/ 0.1 4.10E+19 -2.10 2.62 /

PLOG/ 1.0 7.90E+22 -2.99 16.16 /

PLOG/ 10.0 2.80E+24 -3.33 32.42 /

PLOG/ 100.0 4.70E+18 -1.58 33.47 /

! est C2H5+OH

!

CH2CH2OH+HO2r=CH3CH2OH+O2

1.00E+12 0.00 0.00 !

! est C2H5+HO2

!

CH2CH2OH+HO2r=>CH2OH+CH2O+HOr

3.00E+13 0.00 0.00 !

! est C2H5+HO2

!

CH2CH2OH+O2=HOCH2CH2OO

6.40E+38 -8.77 24.51 ! 1 atm

PLOG/ 0.013 1.50E+44 -11.15 23.11 /

PLOG/ 0.1 4.90E+42 -10.34 24.74 /

PLOG/ 1.0 6.40E+38 -8.77 24.51 /

PLOG/ 10.0 5.60E+32 -6.58 21.11 /

PLOG/ 100.0 4.20E+26 -4.46 16.48 /

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc
Combust Inst 2009 32 271-277

!

CH2CH2OH+O2=CH2CHOH+HO2r

3.60E+13 -0.88 12.86 ! 1 atm

PLOG/ 0.013 1.30E+53 -11.88 150.32 /

PLOG/ 0.1 5.00E+12 -0.79 3.67 /

PLOG/ 1.0 3.60E+13 -0.88 12.86 /

PLOG/ 10.0 4.40E+20 -2.85 35.63 /

PLOG/ 100.0 1.90E+30 -5.51 69.52 /

DUP

CH2CH2OH+O2=CH2CHOH+HO2r

6.00E+03 -10.00 0.83 ! 1 atm
PLOG/ 0.013 2.30E+10 -0.15 -3.31 /
PLOG/ 0.1 2.80E+61 -14.17 181.97 /
PLOG/ 1.0 6.00E+03 -10.00 0.83 /
PLOG/ 10.0 6.00E+03 -10.00 0.83 /
PLOG/ 100.0 6.00E+03 -10.00 0.83 /

DUP

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc
Combust Inst 2009 32 271-277

!

CH2CH2OH+O2=CH2O+CH2O+HO2r

4.40E+24 -4.36 18.39 ! 1 atm
PLOG/ 0.013 5.60E+22 -3.95 5.06 /
PLOG/ 0.1 1.40E+24 -4.31 11.15 /
PLOG/ 1.0 4.40E+24 -4.36 18.39 /
PLOG/ 10.0 3.00E+25 -4.50 28.30 /
PLOG/ 100.0 1.20E+29 -5.44 47.38 /

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc
Combust Inst 2009 32 271-277

!

CH3CH2O(+M)=CH3r+CH2O(+M)

6.30E+10 0.93 71.54 !
LOW/ 4.70E+25 0.93 69.17 /
TROE/ 0.426 0.3 2278.0 100000.0 /

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176-188.

!

CH3CHO+Hr=CH3CH2O

4.60E+07 1.71 29.66 !

! Sivaramakrishnan R Michael JV Klippenstein SJ, J. Phys. Chem. A 114
(2010) 755-764.

!

CH3CH2O+Hr(+M)=CH2OH+CH3r(+M)

2.60E+18 -1.05 21.46 !
LOW/ 3.00E+11 0.89 0.07 /

! Z.F. Xu, K. Xu, M.C. Lin, J. Phys. Chem. A 115 (2011) 3509-3522.

!

CH3CH2O+Hr=CH3CHO+H2

7.50E+09 1.15 2.82 !

! Xu et al., J. Phys. Chem. A 115 (2011) 3509-3522.

!

CH3CH2O+HO2r=CH3CHO+H2O

3.00E+13 0.00 0.00 !

! est

!

CH3CH2O+O2=CH3CHO+HO2r

1.50E+10 0.00 2.70 !

! Fittschen, C.; Frenzel, A.; Imrik, K.; Devolder, P. Int J Chem Kinet
1999, 31, 860-866.

!

CH3CH2O+CO=C2H5r+CO2

9.50E+25 -4.93 37.99 !

! est CH3O+CO=CH3+CO2

!

CH3CHO(+M)=CH3r+HCO(+M)

2.70E+22 -1.74 361.31 !
LOW/ 1.10E+59 -11.30 401.30 /
TROE/ 0.18 462.0 167730.0 1580000.0 /
CO/ 2.14/ CO2/ 2.86/ H2/ 2.86/ N2/ 1.43/ H2O/ 8.57/ CH4/ 4.23/
C2H6/ 4.23/

! Sivaramakrishnan, R.; Michael, J.V.; Klippenstein, S.J. J Phys Chem A
114, 755-764 (2010).

!

CH3CHO=CH2CO+H2

8.50E+44 -9.77 380.35 ! 1 atm
PLOG/ 0.05 4.00E+44 -10.07 365.80 /
PLOG/ 0.1 7.40E+44 -10.05 369.96 /
PLOG/ 1.0 8.50E+44 -9.77 380.35 /
PLOG/ 10.0 2.20E+45 -9.55 396.97 /

! Sivaramakrishnan, R.; Michael, J.V.; Klippenstein, S.J. J Phys Chem A
114, 755-764 (2010).

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J
Phys Chem A 2015, 119, 7724-7733.

!

CH3CHO=CH4+CO

1.90E+45 -9.43 374.11 ! 1 atm
PLOG/ 0.05 5.10E+45 -9.85 372.45 /
PLOG/ 0.1 1.40E+45 -9.65 367.88 /
PLOG/ 1.0 1.90E+45 -9.43 374.11 /
PLOG/ 10.0 1.60E+45 -9.10 388.25 /

! Sivaramakrishnan, R.; Michael, J.V.; Klippenstein, S.J. J Phys Chem A
114, 755-764 (2010).

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J
Phys Chem A 2015, 119, 7724-7733.

!

CH3CHO=CH2CHOH

1.10E+46 -9.76 342.94 ! 1 atm
PLOG/ 0.05 7.30E+45 -10.04 329.64 /
PLOG/ 0.1 2.90E+45 -9.86 330.05 /
PLOG/ 1.0 1.10E+46 -9.76 342.94 /
PLOG/ 10.0 2.80E+45 -9.35 354.15 /

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J
Phys Chem A 2015, 119, 7724-7733.

!

CH3CHO+Hr=CH3CO+H2

1.30E+05 2.58 5.10 !

! R Sivaramakrishnan JV Michael SJ Klippenstein, J. Phys. Chem. A 114
(2010) 755-764.

!

CH3CHO+Hr=CH2CHO+H2

2.70E+03 3.10 21.77 !

! R Sivaramakrishnan JV Michael SJ Klippenstein, J. Phys. Chem. A 114
(2010) 755-764.

!
CH3CHO+Or=CH3CO+HOr
5.80E+12 0.00 7.56 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH3CHO+Or=CH2CHO+HOr
9.00E+04 2.80 24.27 !

! est ½ c2h6+o
!
CH3CHO+HOr=CH3CO+H2O
2.80E+12 0.00 -2.97 !

! S. Wang, D.F. Davidson, R.K. Hanson, Proc. Combust. Inst. 35 (2015)
473-480.

!
CH3CHO+HOr=CH2CHO+H2O
8.50E+13 0.00 22.23 !

! S. Wang, D.F. Davidson, R.K. Hanson, Proc. Combust. Inst. 35 (2015)
473-480.

!
CH3CHO+HO2r=CH3CO+H2O2
1.70E+13 0.00 68.17 !

! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J
Comput Chem 32: 1725-1733, 2011

!
CH3CHO+HO2r=CH2CHO+H2O2
1.10E+13 0.00 97.27 !

! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J
Comput Chem 32: 1725-1733, 2011

!
CH3CHO+O2=CH3CO+HO2r
1.20E+05 2.50 157.13 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH3CHO+O2=CH2CHO+HO2r
1.50E+07 1.90 207.31 !

! est ½ c2h6+o2
!
CH3CHO+CH3r=CH3CO+CH4
3.50E-08 6.21 6.82 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH3CHO+CH3r=CH2CHO+CH4
1.80E-01 3.44 43.45 !

! est ½ c2h6+ch3
!
CH3CHO+CH3O=CH3CO+CH3OH
1.00E+11 0.00 12.47 !

! est ch2o+ch3o
!
CH3CHO+CH3O=CH2CHO+CH3OH
1.20E+11 0.00 29.71 !

! est ½ c2h6+ch3o
!
CH3CHO+CH3OO=CH3CO+CH3OOH
1.70E+13 0.00 68.17 !

! est ch3hco+ho2
!
CH3CHO+CH3OO=CH2CHO+CH3OOH
1.10E+13 0.00 97.27 !

! est ch3hco+ho2
!
CH3CHO+C2H3r_Olef=CH2CHO+C2H4_Olef
2.00E-01 3.96 108.74

! Chen, Song, Song, Lv, Li, Computational and Theoretical Chemistry 1075
(2016) 63-69

!
CH3CHO+C2H3r_Olef=CH3CO+C2H4_Olef
1.60E-01 3.62 70.33

! Chen, Song, Song, Lv, Li, Computational and Theoretical Chemistry 1075
(2016) 63-69

!
cC2H4O=CH2CHO+Hr
1.80E+13 0.20 300.33 !

! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
8016-8027

!
cC2H4O=CH3r+HCO
5.60E+13 0.40 258.91 !

! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
8016-8027

!
cC2H4O=CH3CO+Hr
2.40E+13 0.25 273.26 !

! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
8016-8027

!
cC2H4O=CH2CO+H2
3.60E+12 -0.20 263.72 !

! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
8016-8027

!

cC2H4O=CH3CHO
 3.20E+12 -0.75 194.24 !
 ! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
 8016-8027
 !
cC2H4O=C2H2+H2O
 7.60E+12 0.06 290.91 !
 ! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
 8016-8027
 !
cC2H4O+Hr=CH3CHO+Hr
 5.60E+13 0.00 45.81 !
 ! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005)
 8016-8027
 !
cC2H4O+Hr=cC2H3O+H2
 2.00E+13 0.00 34.77 !
 ! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782
 !
cC2H4O+Hr=C2H3r_Olef+H2O
 5.00E+09 0.00 20.92 !
 ! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782
 !
cC2H4O+Hr=C2H4_Olef+HOr
 9.50E+10 0.00 20.92 !
 ! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782
 !
cC2H4O+Or=cC2H3O+HOr
 1.90E+12 0.00 21.97 !
 ! D.J. Bogan, C.W. Hand, J. Phys. Chem. 82 (1978) 2067
 !
cC2H4O+HOr=cC2H3O+H2O
 1.80E+13 0.00 15.10 !
 ! R.R. Baldwin, A. Keen, R.W. Walker, J. Chem. Soc. Faraday Trans. 80
 (1984) 435
 !
cC2H4O+HO2r=cC2H3O+H2O2
 4.00E+12 0.00 71.13 !
 ! P. Dagaut, D. Voisin, M. Cathonnet, M. McGuinness, J.M. Simmie,
 Combust. Flame 106 (1996) 62-68.
 !
cC2H4O+O2=cC2H3O+HO2r
 4.00E+13 0.00 257.32 !
 ! P. Dagaut, D. Voisin, M. Cathonnet, M. McGuinness, J.M. Simmie,
 Combust. Flame 106 (1996) 62-68.
 !
cC2H4O+CH3r=cC2H3O+CH4
 1.10E+12 0.00 49.50 !

! R.R. Baldwin, A. Keen, R.W. Walker, J. Chem. Soc. Faraday Trans. 80
(1984) 435

!

!CH2CHOH(+M)=CH3CHO(+M) 9.7E23 -3.290 59994 ! see
reverse

! LOW/ 2.9E43 -8.120 52204/

! TROE/ 0.5 863 320 100000/

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176-188.

!

CH2CHOH+Hr=CH2CHO+H2
1.50E+03 3.08 30.25 !

! H-B Rao X-Y Zeng H He Z-R Li J Phys Chem A 2011, 115, 1602-1608

!

CH2CHOH+Hr=CHCHOH+H2
2.50E+07 2.03 63.51 !

! H-B Rao X-Y Zeng H He Z-R Li J Phys Chem A 2011, 115, 1602-1608

!

CH2CHOH+Or=CH2OH+HCO
3.90E+12 0.00 6.25 !

DUP

CH2CHOH+Or=CH2OH+HCO
6.20E+13 0.00 28.68 !

DUP

CH2CHOH+Or=CH2OH+Hr+CO
3.70E+23 -2.47 112.06

DUP

CH2CHOH+Or=CH2OH+Hr+CO
2.30E+22 -2.47 89.63

DUP

! est C2H4+O

!

CH2CHOH+Or=CH2CHO+HOr
1.60E+07 2.00 18.41 !

! est CH3CH2OH+O=CH3CH2O+OH

!

CH2CHOH+HOr=CHCHOH+H2O
1.30E-01 4.20 -3.60 !

! est C2H4+OH

!

CH2CHOH+HOr=CH2CHO+H2O
2.40E+03 2.82 -2.89 !

DUP

CH2CHOH+HOr=CH2CHO+H2O
7.90E+07 1.18 -1.27 !

DUP

! est CH3CH2OH+OH=CH3CH2O+H2O

!

CH2CHOH+HO2r=CH2CHO+H2O2
1.60E+12 0.00 68.17 !

! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J
Comput Chem 32: 1725-1733, 2011

!
CH2CHOH+HO2r=CH3CHO+HO2r
1.50E+05 1.67 28.49 !

! G. da Silva, J.W. Bozzelli, Chem. Phys. Lett. 483 (2009) 25-29 (1 atm)

!
CH2CHOH+O2=>CH2O+HCO+HOr
3.50E+07 1.80 163.18 !

DUP
CH2CHOH+O2=>CH2O+HCO+HOr
-2.10E17 -0.67 246.55

DUP
CH2CHOH+O2=>CH2O+Hr+CO+HOr
2.10E+17 -0.67 246.55

! est C2H4+O2
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016

!
CHCHOH=HCCOH+Hr
1.10E+31 -6.15 214.99 ! 1 atm
PLOG/ 0.04 4.40E+29 -6.15 214.99 /
PLOG/ 1.0 1.10E+31 -6.15 214.99 /
PLOG/ 10.0 1.50E+32 -6.17 218.57 /
PLOG/ 100.0 5.50E+29 -5.06 219.15 /

! Ing W-C Sheng CY Bozzelli JW FPT 83:111-145 2003

!
CHCHOH+Hr=CH2CHO+Hr
5.00E+13 0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
! JAM est

!
CHCHOH+Hr=HCCOH+H2
4.50E+13 0.00 0.00 !

! est C2H3+H

!
CHCHOH+Or=OCHCHO+Hr
5.00E+13 0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
! JAM est

!
CHCHOH+HOr=HCCOH+H2O
2.00E+13 0.00 0.00 !

! est C2H3+OH

!
CHCHOH+O2=OCHCHO+HOr
1.80E+12 0.00 -0.78 !

! c2h2 paper

!

CHCHOH+O2=HOCHO+HCO
3.30E+12 0.00 0.00 !

DUP

CHCHOH+O2=HOCHO+HCO
-1.80E12 0.00 -0.78 !

DUP

CHCHOH+O2=HOCHO+Hr+CO
1.10E+22 -2.50 84.79

! c2h2 paper

!

CHCHOH+CH2O=CH2CHOH+HCO
5.40E+03 2.81 24.52 !

DUP

CHCHOH+CH2O=CH2CHOH+HCO
-3.20E13 0.34 107.89

DUP

CHCHOH+CH2O=CH2CHOH+Hr+CO
3.20E+13 0.34 107.89

! est c2h3+ch2o

!

CHCHOH+HCO=CH2CHOH+CO
9.00E+13 0.00 0.00 !

! est c2h3+hco

!

CHCHOH+CH3r=HCCOH+CH4
2.10E+13 0.00 0.00 !

! est c2h3+ch3

!

cC2H3O=CH2CHO
8.70E+31 -6.90 62.73 !

! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005

!

cC2H3O=CH2CO+Hr
5.00E+13 0.00 62.19 !

! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005

!

cC2H3O=CH3r+CO
7.10E+12 0.00 59.75 !

! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005

!

CH3CO=CH3r+CO
6.50E+18 -2.52 68.77 ! 1 atm
PLOG/ 0.01 6.90E+14 -1.97 61.02 /
PLOG/ 0.025 2.40E+15 -2.00 61.94 /
PLOG/ 0.1 2.00E+16 -2.09 63.58 /
PLOG/ 1.0 6.50E+18 -2.52 68.77 /
PLOG/ 10.0 8.20E+19 -2.55 72.23 /
PLOG/ 100.0 1.30E+20 -2.32 75.36 /

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

!

CH2CO+Hr=CH3CO
 2.30E+08 1.61 10.99 ! (kinf)

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006
 !CH3CO+H=CH3+HCO 2.1E13 0.000 0 !
 ! Bartels M Edelbuttal J Hoyer mann K PCI 23:131 1991
 ! Ohmori K Miyoshi A Matsui H Washida N JPC 94:3253 1990
 ! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
 2016:

CH3CO+Hr=CH3r+HCO
 2.10E+13 0.00 0.00 !

DUP
 CH3CO+Hr=CH3r+HCO
 -1.20E23 -2.47 83.37

DUP
 CH3CO+Hr=CH3r+Hr+CO
 1.20E+23 -2.47 83.37

!
 CH3CO+Hr=CH2CO+H2
 1.20E+13 0.00 0.00 !

! Bartels M Edelbuttal J Hoyer mann K PCI 23:131 1991
 ! Ohmori K Miyoshi A Matsui H Washida N JPC 94:3253 1990
 !

CH3CO+Or=CH3r+CO2
 1.60E+14 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

CH3CO+Or=CH2CO+HOr
 5.30E+13 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

CH3CO+HOr=CH2CO+H2O
 1.20E+13 0.00 0.00 !

! Tsang W Hampson RF JPCRD 15:1087 1986
 !

CH3CO+O2=CH3C(O)OO
 2.80E+34 -7.21 25.36 ! 1 atm
 PLOG/ 0.1 3.60E+31 -4.77 9.15 /
 PLOG/ 1.0 2.80E+34 -7.21 25.36 /
 PLOG/ 10.0 4.90E+31 -6.09 27.37 /

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14,
 1131-1155.
 ! fitted from figure
 !

CH3CO+O2=CH2CO+HO2r
 3.60E+10 0.54 15.57 ! 1 atm
 PLOG/ 0.1 1.30E+08 1.99 0.95 /
 PLOG/ 1.0 3.60E+10 0.54 15.57 /
 PLOG/ 10.0 7.70E+13 -0.34 31.42 /

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14, 1131-1155.

! fitted from figure

!

CH3CO+O2=CH2O+CO+HOr

	4.90E+23	-3.71	24.66	!	1 atm
PLOG/ 0.1	5.10E+22	-3.52	13.62	/	
PLOG/ 1.0	4.90E+23	-3.71	24.66	/	
PLOG/ 10.0	4.80E+22	-3.30	35.97	/	

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14, 1131-1155.

! fitted from figure

!

CH3CO+CH3r=C2H6+CO

	3.30E+13	0.00	0.00	!	
--	----------	------	------	---	--

! Adachi H Basco N James DGL IJCK 13:1251-1276 1981

!

CH3CO+CH3r=CH2CO+CH4

	5.30E+13	0.00	0.00	!	
--	----------	------	------	---	--

! Adachi H Basco N James DGL IJCK 13:1251-1276 1981

!

CH3CO+CH3OO=CH3r+CO2+CH3O

	2.40E+13	0.00	0.00	!	
--	----------	------	------	---	--

! Tsang W Hampson RF JPCRD 15:1087 1986

!

CH2CHO=CH2CO+Hr

	1.30E+34	-6.57	206.92	!	1 atm
PLOG/ 0.01	2.40E+25	-4.80	181.69	/	
PLOG/ 0.1	2.40E+30	-5.86	192.94	/	
PLOG/ 1.0	1.30E+34	-6.57	206.92	/	
PLOG/ 10.0	3.50E+36	-6.92	221.66	/	
PLOG/ 100.0	1.20E+36	-6.48	230.92	/	

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

!

CH2CHO=CH3r+CO

	6.50E+34	-6.87	197.45	!	1 atm
PLOG/ 0.01	1.20E+30	-6.07	172.93	/	
PLOG/ 0.025	1.50E+31	-6.27	177.73	/	
PLOG/ 0.1	6.40E+32	-6.57	185.28	/	
PLOG/ 1.0	6.50E+34	-6.87	197.45	/	
PLOG/ 10.0	2.20E+35	-6.76	207.31	/	
PLOG/ 100.0	2.20E+33	-5.97	211.07	/	

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

!

!CH2CHO+H=CH3+HCO

	1.9E22	-2.300	7693	!	1 atm
! PLOG/ 0.001	1.0E17	-0.903	3024	/	
! PLOG/ 0.010	1.9E17	-0.935	3120	/	
! PLOG/ 0.100	2.5E18	-1.243	4062	/	
! PLOG/ 1.000	1.9E22	-2.300	7693	/	
! PLOG/ 10.00	2.8E25	-3.100	12454	/	
! PLOG/ 100.0	7.5E20	-1.693	13429	/	

! DUP

!CH2CHO+H=CH3+HCO -1.1E32 -4.773 27620 ! 1 atm
! PLOG/ 0.001 0.5E17 -0.903 3024 /
! PLOG/ 1.000E-02 -1.1E27 -3.408 23047 /
! PLOG/ 1.000E-01 -1.5E28 -3.716 23989 /
! PLOG/ 1.000E00 -1.1E32 -4.773 27620 /
! PLOG/ 1.000E01 -1.7E35 -5.573 32381 /
! PLOG/ 1.000E02 -4.5E30 -4.166 33356 /

! DUP

CH2CHO+Hr=CH3r+HCO

1.00E+33 -5.36 71.40 ! 1 atm (refit)
PLOG/ 0.01 5.00E+20 -2.06 16.71 /
PLOG/ 0.1 6.50E+21 -2.37 20.65 /
PLOG/ 1.0 1.00E+33 -5.36 71.40 /
PLOG/ 10.0 1.80E+40 -7.37 102.58 /
PLOG/ 100.0 1.20E+32 -4.93 94.90 /

DUP

CH2CHO+Hr=CH3r+HCO

1.20E+27 -3.85 38.01 ! 1 atm (refit)
PLOG/ 0.01 3.00E+28 -4.17 51.72 /
PLOG/ 0.1 4.00E+29 -4.48 55.66 /
PLOG/ 1.0 1.20E+27 -3.85 38.01 /
PLOG/ 10.0 2.70E+28 -4.08 55.50 /
PLOG/ 100.0 1.97E+24 -2.82 59.85 /

DUP

CH2CHO+Hr=CH3r+Hr+CO

1.10E+32 -4.77 115.56
PLOG/ 0.01 1.10E+27 -3.41 96.43 /
PLOG/ 0.1 1.50E+28 -3.72 100.37 /
PLOG/ 1.0 1.10E+32 -4.77 115.56 /
PLOG/ 10.0 1.70E+35 -5.57 135.48 /
PLOG/ 100.0 4.50E+30 -4.17 139.56 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

! including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

!

CH2CHO+Hr=CH3CO+Hr

9.20E+17 -1.16 34.28 ! 1 atm
PLOG/ 0.001 3.60E+13 0.05 18.00 /
PLOG/ 0.01 4.60E+13 0.02 18.38 /
PLOG/ 0.1 3.40E+14 -0.22 21.39 /
PLOG/ 1.0 9.20E+17 -1.16 34.28 /
PLOG/ 10.0 1.60E+22 -2.27 55.48 /
PLOG/ 100.0 8.10E+19 -1.51 64.99 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!

CH2CHO+Or=CH2O+HCO

5.00E+13 0.00 0.00 !

CH2CHO+Or=CH2O+Hr+CO

3.00E+23 -2.47 83.37

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett. 2016:

```

!
CH2CHO+HOr=CH2CO+H2O
      2.00E+13   0.00 0.00 !

! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
! JAM est
!
CH2CHO+HOr=CH2OH+HCO
      1.00E+13   0.00 0.00 !
CH2CHO+HOr=CH2OH+Hr+CO
      6.00E+22  -2.47 83.37

! JAM est
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016:
!
CH2CHO+HO2r=CH2O+HCO+HOr
      3.10E+13   0.00 0.00 !

! est as C2H5+HO2; prod Marinov NM IJCK 31:183 1999
!
CH2CHO+O2=CH2O+CO+HOr
      7.00E+10   0.00 0.00 !

! E. Delbos, C. Fittschen, H. Hippler, N. Krasteva, M. Olzmann, B.
Viskolcz, J. Phys. Chem. A 110 (2006) 3238-3245.
!
!CH2CHO+CH3=C2H5+CO+H          4.9E14  -0.500      0 ! see
C2H5+HCO
! Marinov NM Pitz WJ Westbrook CK Castaldi MJ Senkan SM CST 116:211 1996
!
CH2CHO+CH2=C2H4_olef+HCO
      5.00E+13   0.00 0.00 !
CH2CHO+CH2=C2H4_olef+Hr+CO
      3.00E+23  -2.47 83.37 !

! JAM est
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
CH2CHO+CH=C2H3r_olef+HCO
      1.00E+14   0.00 0.00 !
CH2CHO+CH=C2H3r_olef+Hr+CO
      6.00E+23  -2.47 83.37 !

! JAM est
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
CHCHO+Hr=CH2CO+Hr
      1.00E+14   0.00 0.00 !

! J.G. Lopez, C.L. Rasmussen, H. Hashemi, M.U. Alzueta, Y. Gao, P.
Marshall, C.F. Goldsmith, P. Glarborg, Int. J. Chem. Kinet. (2016).
! est
!
CHCHO+O2=CO2+Hr+HCO
      2.10E+09   0.99 -1.13 !

```

! J.G. Lopez, C.L. Rasmussen, H. Hashemi, M.U. Alzueta, Y. Gao, P. Marshall, C.F. Goldsmith, P. Glarborg, Int. J. Chem. Kinet. (2016).
! est as CH2+O2

!
CHCHO+O2=OCHCHO+Or
1.30E+06 2.42 6.71 !

! J.G. Lopez, C.L. Rasmussen, H. Hashemi, M.U. Alzueta, Y. Gao, P. Marshall, C.F. Goldsmith, P. Glarborg, Int. J. Chem. Kinet. (2016).
! est as CH2+O2

!
CH2+CO(+M)=CH2CO(+M)
8.10E+11 0.50 18.87 !
LOW/ 2.69E+33 -5.11 29.69 /
TROE/ 0.5907 275.0 1226.0 5185.0 /
N2/ 1.0/ H2O/ 6.0/ AR/ 0.7/

! GRI2.11

!
CH2CO+Hr=CH3r+CO
7.80E+08 1.45 11.63 !

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006 !

!
CH2CO+Hr=HCCO+H2
3.00E+07 2.00 41.84 !

! JAM est

!
CH2CO+Or=CO2+CH2
1.80E+12 0.00 5.65 !

! Washida N Hatakeyama S Takagi H Kyogoku T Sato S JCP 78:4533-4540 1983

!
!CH2CO+O=HCCO+OH 2.0E07 2.000 10000 ! see rv
! JAM est

!
CH2CO+HOr=CH2OH+CO
1.00E+12 0.00 -4.24 !

! Grusdorf J Nolte J Temps F Wagner HGg Ber. Bun. Phys. Chem. 98:546-553
1994

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH2CO+HOr=CH3r+CO2
6.70E+11 0.00 -4.24 !

! Grusdorf J Nolte J Temps F Wagner HGg Ber. Bun. Phys. Chem. 98:546-553
1994

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
CH2CO+HOr=HCCO+H2O
1.00E+07 2.00 12.55 !

! JAM est


```

!
CH2CO+CH2(S)=C2H4_Olef+CO
      1.60E+14   0.00 0.00 !

! Hack W Koch M Wagener R Wagner HGg BBPC 93:165 1989
!
HCCOH+Hr=HCCO+H2
      3.00E+07   2.00 4.18 !

! JAM est
!
!HCCOH+O=HCCO+OH
                                2.0E07   2.000   1900 ! see rv
! JAM est
!
HCCOH+HOr=HCCO+H2O
      1.00E+07   2.00 4.18 !

! JAM est
!
CH+CO(+M)=HCCO(+M)
      5.00E+13   0.00 0.00 !
LOW/  2.70E+28  -3.74 8.10 /
TROE/ 0.5757    237.0 1652.0   5069.0   /
CO/   1.5/ CO2/ 2.0/ H2/  2.0/ N2/  1.0/ H2O/ 6.0/ CH4/ 2.0/
C2H6/ 3.0/ AR/  0.7/

! GRI2.11
!
HCCO+Hr=CH2(S)+CO
      1.50E+14   0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
Troee J Walker RW Warnatz J JPCRD 21:403 1992
!
HCCO+Or=CO+CO+Hr
      1.00E+14   0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Esser C Frank P Just Th Kerr JA Pilling MJ
Troee J Walker RW Warnatz J JPCRD 21:403 1992
!
HCCO+HOr=C2O+H2O
      1.40E+04   2.65 6.16 !

! Xiong et al., Combust. Flame 161 (2014) 885-897
!
HCCO+HOr=CH2CO+Or
      1.30E+06   1.99 47.20 !

! Xiong et al., Combust. Flame 161 (2014) 885-897
!
HCCO+HOr=HCOH+CO
      3.00E+16  -0.94 2.76 ! 1 atm
PLOG/ 1.0     3.00E+16  -0.94 2.76 /
PLOG/ 10.0    1.10E+18  -1.39 5.84 /
PLOG/ 100.0   3.20E+18  -1.52 6.81 /

!PLOG / 100
                                3.8E13   0.050   70/

```

```

! Xiong et al., Combust. Flame 161 (2014) 885-897
! assuming 3-HCOH=1-HCOH=HCOH
DUP
HCCO+HOr=HCOH+CO
      8.70E+19  -1.79 25.08 ! 1 atm
PLOG/ 1.0      8.70E+19  -1.79 25.08 /
PLOG/ 10.0     3.50E+22  -2.48 38.34 /
PLOG/ 100.0    1.30E+24  -2.90 44.02 /

!PLOG / 100                                -6.8E13  0.100  10302/
! Xiong et al., Combust. Flame 161 (2014) 885-897
! assuming 3-HCOH=1-HCOH=HCOH
DUP
HCCO+HOr=HCOH+CO
      2.90E+12   0.37 -0.10

DUP
! Xiong et al., Combust. Flame 161 (2014) 885-897
! assuming 3-HCOH=1-HCOH=HCOH
!
HCCO+HOr=CH2O+CO
      1.20E+21  -2.46 10.58 ! 1 atm

!PLOG / 1                                3.8E13  -0.060  156/
!PLOG / 1                                -2.9E16  -0.800  5071/
!PLOG / 10                               2.1E08   0.030   97/ !results in
negative rate constant
!PLOG / 10                               -1.6E16  -0.720  4883/
!PLOG / 100                              1.1E08   0.110   52/
!PLOG / 100                              -6.4E07  -1.140  6914/
! Xiong et al., Combust. Flame 161 (2014) 885-897
!
HCCO+HOr=OCHCO+Hr
      2.60E+08   1.41 3.55 ! 1 atm
PLOG/ 0.01    2.60E+08   1.41 3.54 /
PLOG/ 0.1     2.60E+08   1.41 3.54 /
PLOG/ 1.0     2.60E+08   1.41 3.55 /
PLOG/ 10.0    3.00E+08   1.40 3.84 /
PLOG/ 100.0   8.20E+08   1.28 6.41 /

! Xiong et al., Combust. Flame 161 (2014) 885-897
!
HCCO+HOr=CO2+CH2
      7.20E+27  -5.02 10.33 ! 1 atm
PLOG/ 0.1     1.70E+15  -1.19 -2.18 /
PLOG/ 1.0     7.20E+27  -5.02 10.33 /
PLOG/ 10.0    1.00E+91  -20.14  480.49 /

!PLOG / 10                                6.0E15  -0.640  363 /
!PLOG / 100                               1.0E14   0.060  447 / !results
in negative rate constant
DUP
HCCO+HOr=CO2+CH2
      1.10E+21  -2.28 70.96 ! 1 atm
PLOG/ 0.1     -7.40E17  -1.92 7.05 /
PLOG/ 1.0     1.10E+21  -2.28 70.96 /
PLOG/ 10.0    2.30E+65  -16.08  81.97 /

```

```

!PLOG / 10                -2.6E19  -1.640    3539 /
!PLOG / 100              -5.6E19  -1.510    5657 /
! Xiong et al., Combust. Flame 161 (2014) 885-897
! ASSUMING 3-CHCOOH = 1-CHCOOH ==fast==> CO2+CH2
DUP
HCCO+HOr=CO2+CH2
    7.10E+19  -2.30 3.45 ! 1 atm
    PLOG/ 0.01  1.00E+19  -2.08 0.18 /
    PLOG/ 0.1   1.40E+19  -2.12 0.37 /
    PLOG/ 1.0   7.10E+19  -2.30 3.45 /
    PLOG/ 10.0  1.80E+20  -2.34 10.13 /

!PLOG / 100                8.2E02   2.870      -3 / !results
in negative rate constant
!PLOG / 100              -2.3E24  -2.700    20416 /
! Xiong et al., Combust. Flame 161 (2014) 885-897
! ASSUMING 3-CHCOOH = 1-CHCOOH ==fast==> CO2+CH2
DUP
HCCO+O2=CO2+CO+Hr
    4.90E+12  -0.14 4.81 !

! Klippenstein SJ Miller JA Harding LB PCI 29:1209-1217 2002
!
HCCO+O2=CO+CO+HOr
    1.60E+11  -0.02 4.27 !

! Klippenstein SJ Miller JA Harding LB PCI 29:1209-1217 2002
!
HCCO+O2=HCO+CO+Or
    2.20E+02   2.69 14.81 !
HCCO+O2=Hr+CO+CO+Or
    1.30E+12   0.22 98.19

! Klippenstein SJ Miller JA Harding LB PCI 29:1209-1217 2002
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett.
2016:
!
HCCO+CH2=C2H3r_Olef+CO
    3.00E+13   0.00 0.00 !

! JAM est
!
HCCO+CH=C2H2+CO
    5.00E+13   0.00 0.00 !

! JAM est
!
HCCO+HCCO=C2H2+CO+CO
    1.00E+13   0.00 0.00 !

! JAM est
!
C2O+M=C+CO+M
    2.00E+15   0.00 184.93 !

! Fridriechs, G.; Wagner, H.Gg. Z. Phys. Chem. 203, 1-14, 1998.
!
```

C2O+Hr=CH+CO
 1.30E+13 0.00 0.00 !

 ! Bauer W Becker KH Meuser R BBPC 89:340 1985
 !
 C2O+Or=CO+CO
 5.20E+13 0.00 0.00 !

 ! Bauer W Becker KH Meuser R BBPC 89:340 1985
 !
 C2O+HOr=CO+CO+Hr
 2.00E+13 0.00 0.00 !

 ! JAM est
 !
 C2O+O2=CO+CO+Or
 1.00E+13 0.00 10.88 !

 ! Becker KH Konig R Meuser R Wiesen P Bayes KD J Photochem Photobiol A
 64:1-14 1992
 ! Williamson DG Bayes KD JACS 89:3390 1967
 !
 C2O+O2=CO+CO2
 1.00E+13 0.00 10.88 !

 ! Becker KH Konig R Meuser R Wiesen P Bayes KD J Photochem Photobiol A
 64:1-14 1992
 ! Williamson DG Bayes KD JACS 89:3390 1967
 !
 C2O+C=CO+C2
 1.00E+14 0.00 0.00 !

 ! Fridriechs, G.; Wagner, H.Gg. Z. Phys. Chem. 203, 1-14, 1998.
 !
 !
 CH3CH2OOH=CH3CH2O+HOr
 9.30E+52 -11.91 223.33 ! 1 atm
 PLOG/ 0.1 6.10E+58 -14.05 226.48 /
 PLOG/ 1.0 9.30E+52 -11.91 223.33 /
 PLOG/ 100.0 1.40E+33 -5.27 203.74 /

! (300-1000 K) from D. Chen et al., J. Phys. Chem. A 115 (2011) 602-611.
 !
 CH3CH2OOH+Hr=CH3CHOOH+H2
 6.50E+10 0.00 7.78

 ! est CH3OOH+H
 !
 CH3CH2OOH+Hr=CH3CH2OO+H2
 4.30E+10 0.00 7.78

 ! est CH3OOH+H
 !
 CH3CH2OOH+Hr=CH3CH2O+H2O
 1.20E+10 0.00 7.78

 ! est CH3OOH+H
 !

```

CH3CH2OOH+Or=CH3CHOOH+HOr
    1.60E+13    0.00 19.87

! est CH3OOH+O
!
CH3CH2OOH+Or=CH3CH2OO+HOr
    8.70E+12    0.00 19.87

! est CH3OOH+O
!
CH3CH2OOH+HOr=CH3CHOOH+H2O
    7.20E+11    0.00 -1.08

! est CH3OOH+OH
!
CH3CH2OOH+HOr=CH3CH2OO+H2O
    1.10E+12    0.00 -1.83

! est CH3OOH+OH
!
CH3CH2OOH+HO2r=CH3CH2OO+H2O2
4.10E+04    2.50 42.70

! est CH2O+HO2
!
CH3CHOOH=CH3CHO+HOr
    3.50E+12   -0.95 4.10 ! 1 atm
PLOG/ 1.0    3.50E+12   -0.95 4.10 /
PLOG/ 10.0   3.50E+13   -0.95 4.10 /
PLOG/ 100.0  5.80E+14   -1.01 4.47 /

! RAS/GLA08b ING/BOZ03
!
CH3CH2OO=CH2CH2OOH
    1.30E+17   -2.81 119.24 ! 1 atm
PLOG/ 1.0E-4   3.20E+31   -8.25 122.84 /
PLOG/ 3.0E-4   3.50E+30   -7.88 122.72 /
PLOG/ 0.001   1.50E+29   -7.37 122.21 /
PLOG/ 0.003   3.50E+27   -6.77 121.34 /
PLOG/ 0.01    3.60E+25   -6.04 120.42 /
PLOG/ 0.03    1.60E+24   -5.51 120.50 /
PLOG/ 0.1     1.40E+21   -4.40 118.87 /
PLOG/ 0.3     2.90E+19   -3.73 119.20 /
PLOG/ 1.0     1.30E+17   -2.81 119.24 /
PLOG/ 3.0     5.30E+14   -1.90 119.12 /
PLOG/ 10.0    4.70E+13   -1.40 121.21 /
PLOG/ 30.0    4.20E+12   -0.92 122.93 /
PLOG/ 100.0   1.90E+08    0.57 119.62 /

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.
!
CH3CH2OO=C2H4_Olef+HO2r
    8.70E+39   -9.01 158.07 ! 1 atm
PLOG/ 1.0E-4   1.90E+46   -11.85 152.46 /
PLOG/ 3.0E-4   4.20E+46   -11.88 154.05 /
PLOG/ 0.001   3.60E+46   -11.77 155.23 /
PLOG/ 0.003   1.70E+46   -11.58 156.19 /
PLOG/ 0.01    4.40E+45   -11.28 157.19 /

```

PLOG/ 0.03	8.10E+44	-10.94	158.07	/
PLOG/ 0.1	4.60E+43	-10.43	158.62	/
PLOG/ 0.3	8.70E+41	-9.77	158.41	/
PLOG/ 1.0	8.70E+39	-9.01	158.07	/
PLOG/ 3.0	7.20E+36	-7.95	155.81	/
PLOG/ 10.0	4.30E+33	-6.84	153.39	/
PLOG/ 30.0	1.90E+30	-5.71	150.25	/
PLOG/ 100.0	1.60E+26	-4.37	145.77	/

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

CH3CH2OO=cC2H4O+HO_r

	1.50E+44	-10.71	180.08	! 1 atm	
PLOG/ 1.0E-4		2.00E+49	-13.32	162.42	/
PLOG/ 3.0E-4		1.70E+50	-13.52	165.31	/
PLOG/ 0.001	6.60E+50	-13.62	168.11		/
PLOG/ 0.003	3.90E+48	-12.85	166.65		/
PLOG/ 0.01	7.60E+48	-12.82	169.95		/
PLOG/ 0.03	9.70E+46	-12.11	170.04		/
PLOG/ 0.1	9.90E+46	-11.94	174.35		/
PLOG/ 0.3	1.30E+45	-11.20	175.81		/
PLOG/ 1.0	1.50E+44	-10.71	180.08		/
PLOG/ 3.0	1.00E+42	-9.86	182.59		/
PLOG/ 10.0	2.50E+39	-8.87	185.31		/
PLOG/ 30.0	1.90E+36	-7.75	186.86		/
PLOG/ 100.0	2.50E+31	-6.10	186.44		/

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

CH3CH2OO+H_r=CH3CH2O+HO_r

	9.60E+13	0.00	0.00
--	----------	------	------

! est CH3OO+H

!

CH3CH2OO+O_r=CH3CH2O+O2

	2.90E+10	1.00	-3.03
--	----------	------	-------

! est CH3OO+O

!

CH3CH2OO+HO_r=CH3CH2OH+O2

	5.10E+15	-0.81	0.00
--	----------	-------	------

! est CH3OO+OH

!

CH3CH2OO+HO2_r=CH3CH2OOH+O2

	3.60E+11	0.00	-5.30
--	----------	------	-------

! Noell et al., J. Phys. Chem. A 2010, 114, 6983-6995 (221-296 K)

!

CH3CH2OO+CO=CH3CH2O+CO2

	1.60E+05	2.18	75.06
--	----------	------	-------

! est CH3OO+CO

!

CH3CH2OO+CH3_r=CH3CH2O+CH3O

	5.10E+12	0.00	-5.90
--	----------	------	-------

! est CH3OO+CH3

```

!
CH3CH2OO+CH4=CH3CH2OOH+CH3r
      1.20E+01    3.69 89.12

! H-H Carstensen, A.M. Dean, O. Deutschmann, Proc. Combust. Inst. 31
(2007) 149-157
!
CH3CH2OO+CH3OH=CH3CH2OOH+CH2OH
      4.00E+13    0.00 81.17

! est CH3OO+CH3OH
!
CH3CH2OO+CH2O=CH3CH2OOH+HCO
      4.10E+04    2.50 42.70
CH3CH2OO+CH2O=CH3CH2OOH+Hr+CO
      2.50E+14    0.03 126.08

! est CH3OO+CH2O
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
CH3CH2OO+C2H6=CH3CH2OOH+C2H5r
      8.60E+00    3.76 71.96

! Carstensen H-H Dean AM PCI 30:995-1003 2005
!
CH3CH2OO+C2H5r=CH3CH2O+CH3CH2O
      5.10E+12    0.00 -5.90

! est CH3OO+CH3
!
CH3CH2OO+CH3CHO=CH3CH2OOH+CH3CO
      1.70E+13    0.00 68.17

! est CH3CHO+HO2
!
CH3CH2OO+CH3CHO=CH3CH2OOH+CH2CHO
      1.10E+13    0.00 97.27

! est CH3CHO+HO2
!
CH3CH2OO+CH3CH2OO=CH3CH2O+CH3CH2O+O2
      2.20E+10    0.00 0.19

! Noell et al., J. Phys. Chem. A 2010, 114, 6983-6995 (221-296 K)
!
CH3CH2OO+CH3CH2OO=CH3CHO+CH3CH2OH+O2
      5.60E+10    0.00 0.19

! Noell et al., J. Phys. Chem. A 2010, 114, 6983-6995 (221-296 K)
!
! CH2CH2OOH=C2H5+O2          1          1          1
! see the reverse
!
CH2CH2OOH=cC2H4O+HOr
      2.00E+31   -6.53 73.43
      PLOG/ 1.0E-4      2.20E+24   -5.76 51.92 /
      PLOG/ 3.0E-4      7.30E+26   -6.39 55.81 /

```

PLOG/ 0.001	1.30E+29	-6.91	59.58	/
PLOG/ 0.003	1.70E+28	-6.45	59.54	/
PLOG/ 0.01	2.20E+30	-6.94	63.68	/
PLOG/ 0.03	1.40E+30	-6.70	65.02	/
PLOG/ 0.1	1.00E+32	-7.10	69.50	/
PLOG/ 0.3	6.30E+31	-6.87	71.46	/
PLOG/ 1.0	2.00E+31	-6.53	73.43	/
PLOG/ 3.0	1.20E+30	-6.00	74.27	/
PLOG/ 10.0	4.00E+27	-5.08	73.43	/
PLOG/ 30.0	7.80E+24	-4.12	71.67	/
PLOG/ 100.0	3.20E+21	-2.97	68.62	/

! Klippenstein SJ.Proc Combust Inst 2017;36:77-111.

!

CH2CHOOH=CH2CHO+HOr

	2.00E+35	-6.70	198.53	! 1 atm
PLOG/ 1.0	2.00E+35	-6.70	198.53	/
PLOG/ 10.0	1.10E+28	-4.15	193.26	/
PLOG/ 50.0	2.80E+26	-3.50	193.89	/
PLOG/ 100.0	2.20E+17	-0.42	186.70	/

! est CH3OOH

!

CH2CHOOH+Hr=CH2CHOO+H2

	4.30E+10	0.00	7.78
--	----------	------	------

! est CH3OOH+H

CH2CHOOH+Hr=CH2CHO+H2O

	1.20E+10	0.00	7.78
--	----------	------	------

! est CH3OOH+H

CH2CHOOH+Or=CH2CHOO+HOr

	8.70E+12	0.00	19.87
--	----------	------	-------

! est CH3OOH+O

CH2CHOOH+HOr=CH2CHOO+H2O

	1.10E+12	0.00	-1.83
--	----------	------	-------

! est CH3OOH+OH

CH2CHOOH+HO2r=CH2CHOO+H2O2

	4.10E+04	2.50	42.70
--	----------	------	-------

! est CH2O+HO2

CH2CHOO=CHCHO+HOr

	3.80E+46	-10.72	217.15	! 1 atm
PLOG/ 0.01	3.60E+49	-12.13	282.09	/
PLOG/ 0.1	1.40E+36	-9.92	172.46	/
PLOG/ 0.316	4.20E+40	-10.53	182.72	/
PLOG/ 1.0	3.80E+46	-10.72	217.15	/
PLOG/ 3.16	1.60E+49	-11.24	226.56	/
PLOG/ 10.0	2.40E+51	-11.64	238.40	/
PLOG/ 31.6	2.00E+54	-12.22	258.74	/
PLOG/ 100.0	9.50E+195	-52.27	684.08	/

DUP

CH2CHOO=CHCHO+HOr

	2.30E+124	-36.77	293.30	! 1 atm
PLOG/ 0.01	1.20E+56	-14.81	253.97	/
PLOG/ 0.1	2.30E+40	-9.39	210.96	/

PLOG/ 0.316 1.60E+43 -9.99 210.41 /
PLOG/ 1.0 2.30E+124 -36.77 293.30 /
PLOG/ 3.16 1.90E+103 -29.49 273.68 /
PLOG/ 10.0 6.00E+86 -23.81 260.12 /
PLOG/ 31.6 1.50E+57 -13.94 231.75 /
PLOG/ 100.0 1.80E+34 -6.40 209.20 /

DUP

!

CH2CHOO=CH2CHO+Or

7.60E+81 -21.28 272.29 ! 1 atm
PLOG/ 0.01 2.70E+180 -48.19 708.35 /
PLOG/ 0.1 3.90E+38 -8.69 178.95 /
PLOG/ 0.316 4.60E+47 -11.21 196.86 /
PLOG/ 1.0 7.60E+81 -21.28 272.29 /
PLOG/ 3.16 1.90E+68 -16.83 253.89 /
PLOG/ 10.0 2.00E+55 -12.69 233.63 /
PLOG/ 31.6 1.10E+53 -11.79 237.19 /
PLOG/ 100.0 4.30E+48 -10.31 234.68 /

DUP

CH2CHOO=CH2CHO+Or

2.40E+33 -6.62 172.72 ! 1 atm
PLOG/ 0.01 1.50E+30 -6.64 172.00 /
PLOG/ 0.1 9.70E-12 5.96 95.77 /
PLOG/ 0.316 4.00E+22 -3.71 151.75 /
PLOG/ 1.0 2.40E+33 -6.62 172.72 /
PLOG/ 3.16 6.40E+31 -5.96 172.63 /
PLOG/ 10.0 2.10E+29 -5.10 170.33 /
PLOG/ 31.6 4.70E+27 -4.50 169.58 /
PLOG/ 100.0 6.00E+25 -3.85 167.86 /

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779

!

CH2CHOO=OCHCHO+Hr

1.50E+44 -10.12 170.67 ! 1 atm
PLOG/ 0.01 6.40E+80 -22.20 216.52 /
PLOG/ 0.1 3.30E+65 -17.01 201.21 /
PLOG/ 0.316 6.00E+51 -12.62 179.91 /
PLOG/ 1.0 1.50E+44 -10.12 170.67 /
PLOG/ 3.16 1.30E+59 -14.33 215.02 /
PLOG/ 10.0 4.90E+26 -4.67 143.59 /
PLOG/ 31.6 2.10E+33 -6.38 165.35 /
PLOG/ 100.0 1.30E+32 -5.92 170.12 /

DUP

CH2CHOO=OCHCHO+Hr

1.60E+19 -2.82 115.56 ! 1 atm
PLOG/ 0.01 1.20E+28 -6.01 120.25 /
PLOG/ 0.1 1.40E+25 -4.80 121.08 /
PLOG/ 0.316 2.90E+20 -3.29 115.27 /
PLOG/ 1.0 1.60E+19 -2.82 115.56 /
PLOG/ 3.16 1.90E+22 -3.54 125.44 /
PLOG/ 10.0 7.50E+29 -5.75 144.31 /
PLOG/ 31.6 7.10E+61 -16.16 181.08 /
PLOG/ 100.0 1.10E+19 -2.56 124.14 /

DUP

!

CH2CHOO=CH2CO+HOr
 1.50E+19 -3.61 180.16 ! 1 atm
 PLOG/ 0.01 1.20E+47 -12.28 315.18 /
 PLOG/ 0.1 8.40E+09 -2.06 141.08 /
 PLOG/ 0.316 6.10E+04 0.17 143.18 /
 PLOG/ 1.0 1.50E+19 -3.61 180.16 /
 PLOG/ 3.16 2.10E+33 -7.39 215.94 /
 PLOG/ 10.0 4.40E+36 -7.99 228.78 /
 PLOG/ 31.6 1.20E+37 -7.80 236.23 /
 PLOG/ 100.0 9.10E+35 -7.21 240.79 /

DUP

CH2CHOO=CH2CO+HOr
 3.20E+27 -7.76 155.77 ! 1 atm
 PLOG/ 0.01 2.30E+02 -0.73 107.57 /
 PLOG/ 0.1 1.80E-23 7.84 84.47 /
 PLOG/ 0.316 3.80E+63 -20.44 181.67 /
 PLOG/ 1.0 3.20E+27 -7.76 155.77 /
 PLOG/ 3.16 2.30E-05 3.47 132.05 /
 PLOG/ 10.0 1.10E-01 2.64 142.93 /
 PLOG/ 31.6 5.60E+02 1.70 152.51 /
 PLOG/ 100.0 1.10E+07 0.52 161.80 /

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779
 !

CH2CHOO=CH2O+HCO
 8.60E+33 -6.88 143.80 ! 1 atm
 PLOG/ 0.01 1.70E+174 -55.52 252.38 /
 PLOG/ 0.1 9.00E+66 -17.25 201.33 /
 PLOG/ 0.316 1.80E+43 -9.87 158.82 /
 PLOG/ 1.0 8.60E+33 -6.88 143.80 /
 PLOG/ 3.16 7.30E+171 -43.53 802.91 /
 PLOG/ 10.0 1.00E+32 -6.06 148.53 /
 PLOG/ 31.6 1.90E+34 -6.57 161.13 /
 PLOG/ 100.0 5.70E+29 -5.19 153.97 /

DUP

CH2CHOO=CH2O+HCO
 1.10E+130 -39.38 228.86 ! 1 atm
 PLOG/ 0.01 2.30E+35 -7.97 130.88 /
 PLOG/ 0.1 2.10E+26 -4.96 120.42 /
 PLOG/ 0.316 1.50E+20 -3.08 111.42 /
 PLOG/ 1.0 1.10E+130 -39.38 228.86 /
 PLOG/ 3.16 2.40E+34 -6.87 149.37 /
 PLOG/ 10.0 2.20E+175 -53.78 286.60 /
 PLOG/ 31.6 1.10E+185 -54.22 372.33 /
 PLOG/ 100.0 4.70E+02 1.81 75.73 /

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779
 ! assume 70% HCO

CH2CHOO=CH2O+Hr+CO
 2.00E+34 -6.88 143.80 ! 1 atm
 PLOG/ 0.01 3.90E+174 -55.52 252.38 /
 PLOG/ 0.1 2.10E+67 -17.25 201.33 /
 PLOG/ 0.316 4.30E+43 -9.87 158.82 /
 PLOG/ 1.0 2.00E+34 -6.88 143.80 /
 PLOG/ 3.16 1.70E+172 -43.53 802.91 /

PLOG/ 10.0 2.40E+32 -6.06 148.53 /
PLOG/ 31.6 4.30E+34 -6.57 161.13 /
PLOG/ 100.0 1.30E+30 -5.19 153.97 /

DUP

CH2CHOO=CH2O+Hr+CO

2.50E+130 -39.38 228.86 ! 1 atm
PLOG/ 0.01 5.30E+35 -7.97 130.88 /
PLOG/ 0.1 4.90E+26 -4.96 120.42 /
PLOG/ 0.316 3.40E+20 -3.08 111.42 /
PLOG/ 1.0 2.50E+130 -39.38 228.86 /
PLOG/ 3.16 5.50E+34 -6.87 149.37 /
PLOG/ 10.0 5.10E+175 -53.78 286.60 /
PLOG/ 31.6 2.50E+185 -54.22 372.33 /
PLOG/ 100.0 1.10E+03 1.81 75.73 /

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779

! assume 30% H+CO

!

CH2CHOO=CO+CH3O

3.80E+33 -7.20 146.86 ! 1 atm
PLOG/ 0.01 5.20E+33 -7.92 131.04 /
PLOG/ 0.1 1.30E+98 -27.09 268.03 /
PLOG/ 0.316 1.80E+33 -7.27 141.25 /
PLOG/ 1.0 3.80E+33 -7.20 146.86 /
PLOG/ 3.16 1.30E+79 -19.61 313.26 /
PLOG/ 10.0 4.10E+32 -6.62 155.69 /
PLOG/ 31.6 6.90E+44 -10.04 196.77 /
PLOG/ 100.0 2.90E+01 2.49 90.83 /

DUP

CH2CHOO=CO+CH3O

1.20E-39 13.61 -5.51 ! 1 atm
PLOG/ 0.01 2.30E+129 -41.86 191.84 /
PLOG/ 0.1 2.40E+28 -5.99 127.78 /
PLOG/ 0.316 8.70E-50 16.63 -16.32 /
PLOG/ 1.0 1.20E-39 13.61 -5.51 /
PLOG/ 3.16 8.80E+86 -23.08 255.27 /
PLOG/ 10.0 1.30E+03 1.44 78.07 /
PLOG/ 31.6 2.00E+17 -2.23 119.62 /
PLOG/ 100.0 2.90E+01 2.49 90.83 /

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779

!

CH2CHOO=CO2+CH3r

3.30E+33 -7.22 146.40 ! 1 atm
PLOG/ 0.01 5.10E+33 -7.95 130.92 /
PLOG/ 0.1 1.20E+118 -33.13 308.74 /
PLOG/ 0.316 8.60E+32 -7.21 140.37 /
PLOG/ 1.0 3.30E+33 -7.22 146.40 /
PLOG/ 3.16 3.50E-79 25.01 -87.95 /
PLOG/ 10.0 8.20E+32 -6.76 155.94 /
PLOG/ 31.6 7.00E+37 -8.06 176.56 /
PLOG/ 100.0 6.70E+48 -11.66 184.43 /

DUP

CH2CHOO=CO2+CH3r

1.80E-47 15.85 -22.10 ! 1 atm
PLOG/ 0.01 4.20E+122 -39.75 182.59 /

PLOG/ 0.1	2.00E+29	-6.29	129.37	/
PLOG/ 0.316	5.10E-66	21.37	-46.48	/
PLOG/ 1.0	1.80E-47	15.85	-22.10	/
PLOG/ 3.16	3.80E+32	-6.80	149.33	/
PLOG/ 10.0	4.60E+00	2.10	71.84	/
PLOG/ 31.6	3.50E+14	-1.58	110.75	/
PLOG/ 100.0	1.90E+03	2.08	105.09	/

DUP

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779

!

CH2CHOO+Hr=CH2CHO+HOr
 9.60E+13 0.00 0.00 !

! est CH3OO+H=CH3O+OH

!

CH2CHOO+Or=CH2CHO+O2
 1.60E+13 0.00 -0.61 !

! est CH3OO+O=CH3O+O2

!

CH2CHOO+HOr=CH2CHOH+O2
 2.00E+15 -0.60 0.00 !

! est CH3OO+OH=CH3OH+O2

!

CH2CHOO+HOr=CH2CHO+HO2r
 4.00E+11 0.60 0.00 !

! est H3OO+OH=CH3O+HO2

!

CH2CHOO+HO2r=CH2CHOOH+O2
 4.50E+11 0.00 -5.82 !

! est CH3CH2OO+HO2

! est CH3OO+CO=CH3O+CO2

!

!

CH2CHOO+CO=CH2CHO+CO2
 1.60E+05 2.18 75.06 !

CH2CHOO+CH3r=CH2CHO+CH3O
 5.10E+12 0.00 -5.90 !

! est CH3OO+CH3=CH3O+CH3O

!

CH2CHOO+CH4=CH2CHOOH+CH3r
 4.70E+04 2.50 87.86 !

! est CH4+HO2=CH3+H2O2

!

CH2CHOO+CH3OH=CH2CHOOH+CH2OH
 4.00E+13 0.00 81.17 !

! est CH3OO+CH3OH=CH3OOH+CH2OH

!

CH2CHOO+CH2O=CH2CHOOH+HCO
 4.10E+04 2.50 42.70 !

! est CH3OO+CH2O=CH3OOH+HCO
!
CH2CHOO+C2H6=CH2CHOOH+C2H5r
8.60E+00 3.76 71.96 !

! est=CH3CH2OO+C2H6
!
!
OCHCHO=CH2O+CO

	8.00E+55	-12.60	320.97	!1.0 bar, 800 K < T < 2500 K	
PLOG/	0.009869	4.20E+53	-12.50	296.42	/
PLOG/	0.04935	5.10E+54	-12.60	305.48	/
PLOG/	0.09869	1.00E+55	-12.60	309.10	/
PLOG/	0.4935	4.50E+55	-12.60	317.44	/
PLOG/	0.9869	8.00E+55	-12.60	320.97	/
PLOG/	4.935	1.10E+56	-12.20	324.86	/
PLOG/	9.869	5.50E+56	-12.60	334.57	/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem.
Chem. Phys. 10 (2008) 6520-6533.

!
OCHCHO=HCOH+CO

	2.60E+57	-13.20	333.69	! 1.0 bar, 800 K < T < 2500	
K					
PLOG/	0.009869	8.40E+52	-12.60	302.89	/
PLOG/	0.04935	8.30E+54	-12.90	314.27	/
PLOG/	0.09869	4.40E+55	-13.00	319.06	/
PLOG/	0.4935	1.30E+57	-13.20	329.91	/
PLOG/	0.9869	2.60E+57	-13.20	333.69	/
PLOG/	4.935	1.00E+57	-12.90	339.58	/
PLOG/	9.869	5.70E+59	-13.30	349.53	/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem.
Chem. Phys. 10 (2008) 6520-6533.

!
OCHCHO=CO+CO+H2

	6.10E+57	-13.10	335.34	! 1.0 bar, 800 K < T < 2500 K	
PLOG/	0.009869	6.00E+51	-12.10	300.64	/
PLOG/	0.04935	1.40E+54	-12.50	312.76	/
PLOG/	0.09869	1.80E+55	-12.70	318.56	/
PLOG/	0.4935	1.30E+57	-13.00	330.42	/
PLOG/	0.9869	6.10E+57	-13.10	335.34	/
PLOG/	4.935	5.80E+57	-12.90	342.55	/
PLOG/	9.869	3.40E+59	-13.30	352.69	/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem.
Chem. Phys. 10 (2008) 6520-6533.

!
OCHCHO=HCO+HCO

	1.90E+57	-12.80	352.80	! 1.0 bar, 800 K < T < 2500	
K					
PLOG/	0.009869	1.00E+42	-9.70	307.67	/
PLOG/	0.04935	6.00E+48	-11.10	324.10	/
PLOG/	0.09869	1.70E+51	-11.60	331.00	/
PLOG/	0.4935	5.30E+55	-12.50	346.33	/
PLOG/	0.9869	1.90E+57	-12.80	352.80	/
PLOG/	4.935	2.20E+59	-13.10	365.09	/

PLOG/ 9.869 3.00E+60 -13.30 372.35 /

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem. Chem. Phys. 10 (2008) 6520-6533.
!

OCHCHO+Hr=CH2O+HCO
5.40E+13 0.00 17.99 !

OCHCHO+Hr=CH2O+Hr+CO
3.20E+23 -2.47 101.37

! Colberg, M., Friedrichs, G. J. Phys. Chem. A 110 (2006) 160-170.
! applying prompt HCO dissociation - Labbe et al., J. Phys. Chem. Lett. 2016:
!

OCHCHO+Or=OCHCO+HOr
4.20E+11 0.57 11.55 !

! est CH2O+O
!

OCHCHO+HOr=OCHCO+H2O
4.00E+06 2.00 -6.82 !

! Feierabend, K.J., Zhu, L., Talukdar, R.K., Burkholder, J.B. J. Phys. Chem. A 112 (2008) 73-82.
!

!OCHCHO+HO2=>HOCH(OO)CHO 1.3E31 -7.532 1440 !
!HOCH(OO)CHO => OCHCHO+HO2 1.9E29 -5.781 15790 !
!HOCH(OO)CHO => HOCHO+CO+OH 1.6E10 0.051 15190 !
! da Silva, G. J. Phys. Chem. A 115 (2011) 191-197.
!

OCHCHO+HO2r=HOCHO+CO+HOr
3.30E-04 4.00 1.26 !

! da Silva, G. J. Phys. Chem. A 115 (2011) 191-197.
!

OCHCHO+HO2r=OCHCO+H2O2
4.10E+04 2.50 42.70 !

! est CH2O+HO2
!

OCHCHO+O2=OCHCO+HO2r
2.40E+05 2.50 152.55 !

! est CH2O+O2
!

OCHCO=HCO+CO
4.10E+14 0.00 36.67 ! 1.0 atm
PLOG/ 0.01 3.80E+12 0.00 36.02 /
PLOG/ 0.01 -8.00E21 -2.36 114.73 /
PLOG/ 0.1 3.80E+13 0.00 36.25 /
PLOG/ 1.0 4.10E+14 0.00 36.67 /
PLOG/ 100.0 1.10E+14 0.13 42.43 /

! kinf 1.1E14 0.133 10140 !

OCHCO=Hr+CO+CO
2.50E+24 -2.47 120.05 ! 1 atm
PLOG/ 0.01 8.00E+21 -2.36 114.73 /
PLOG/ 0.1 2.30E+23 -2.47 119.63 /

```

PLOG/ 1.0    2.50E+24  -2.47 120.05    /
PLOG/ 100.0  1.40E+24  -2.42 129.67    /

! da Silva, G. Phys. Chem. Chem. Phys. 12 (2010) 6698-6705.
! including prompt dissociation of HCO (following Labbe et al., J. Phys.
Chem. Lett. 2016)
!
OCHCO+O2=CO+CO2+HOr
      3.30E+14    0.00 8.68 ! 1.0 atm
PLOG/ 0.01    1.60E+14    0.00 6.44 /
PLOG/ 0.1     1.10E+14    0.00 5.44 /
PLOG/ 1.0     3.30E+14    0.00 8.68 /

! kinf                                3.4E04    1.929    344 !
! da Silva, G. Phys. Chem. Chem. Phys. 12 (2010) 6698-6705.
!
HOCHO(+M)=CO+H2O(+M)
      7.50E+14    0.00 287.48    !
LOW/   4.10E+15    0.00 221.67    /

! J.-G. Chang, H.-T. Chen, S. Xu, M.C. Lin, J. Phys. Chem. A 111 (2007)
6789-6797.
!
HOCHO(+M)=CO2+H2(+M)
      4.50E+13    0.00 285.52    !
LOW/   1.70E+15    0.00 213.84    /

! J.-G. Chang, H.-T. Chen, S. Xu, M.C. Lin, J. Phys. Chem. A 111 (2007)
6789-6797.
!
HOCHO+Hr=HOCO+H2
      2.30E+02    3.27 20.33 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+Hr=OCHO+H2
      4.20E+05    2.25 58.96 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
!HOCHO+H=HOCHOH                                2.5E05    2.357    9783 !
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+Or=HOCO+HOr
      5.10E+01    3.42 17.64 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+Or=OCHO+HOr
      1.70E+05    2.10 41.34 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+HOr=HOCO+H2O
      7.80E-06    5.57 -9.90 !

! J.M. Anglada, J. Am. Chem. Soc. 126 (2004) 9809-9820.
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

```

!
 HOCHO+HO2r=OCHO+H2O
 4.90E-05 4.91 -21.20 !

 ! J.M. Anglada, J. Am. Chem. Soc. 126 (2004) 9809-9820.
 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 HOCHO+HO2r=HOCO+H2O2
 4.70E-01 3.98 70.24 !

 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 HOCHO+HO2r=OCHO+H2O2
 3.90E+01 3.08 105.46 !

 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 HOCO+HO2r=HOCHO+O2
 4.00E+11 0.00 0.00 !

 ! H.G. Yu, G. Poggi, J.S. Francisco, J.T. Muckerman, J. Chem. Phys. 129
 (2008) 214307.
 !
 HOCHO+O2=OCHO+HO2r
 3.00E+13 0.00 263.59 !

 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 OCHO=CO2+Hr
 1.00E+10 0.00 0.00 !

 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 OCHO+O2=CO2+HO2r
 5.00E+13 0.00 0.00 !

 ! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
 !
 HOCH2CH2OO=CH2O+CH2O+HO2r
 2.00E+15 -2.03 66.58 ! 1 atm
 PLOG/ 0.013 5.60E+13 -1.90 59.99 /
 PLOG/ 0.1 2.20E+14 -1.92 62.22 /
 PLOG/ 1.0 2.00E+15 -2.03 66.58 /
 PLOG/ 10.0 5.00E+16 -2.26 73.44 /
 PLOG/ 100.0 3.80E+18 -2.60 83.56 /

 ! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc
 Combust Inst 2009 32 271-277
 !
 HOCH2CH2OO=CH2CHOH+HO2r
 1.40E+10 -0.78 62.07 ! 1 atm
 PLOG/ 0.013 2.00E+09 -1.01 55.06 /
 PLOG/ 0.1 2.10E+09 -0.81 56.89 /
 PLOG/ 1.0 1.40E+10 -0.78 62.07 /
 PLOG/ 10.0 8.50E+11 -1.01 71.32 /
 PLOG/ 100.0 5.80E+14 -1.51 86.03 /

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc
Combust Inst 2009 32 271-277

!
HOCH2CH2OO+HO2r=>CH2OOH+CH2OH+O2
2.50E+11 0.00 -6.23 !

!HOCH2CH2OO+HO2=HOCH2CH2OOH+O2 2.5E11 0.000 -1490 !
! est CH3OO+HO2 (CK no 4 products)

!
HOCH2CH2OO+CH2O=>CH2OOH+CH2OH+HCO
4.10E+04 2.50 42.70 !

!HOCH2CH2OO+CH2O=>HOCH2CH2OOH+HCO 4.1E04 2.500 10206 !
! est=CH2O+HO2

!
HOCH2CH2OO+C2H4_olef=>CH2O+CH2OH+CH3CHO
2.20E+12 0.00 71.96 !

!HOCH2CH2OO+C2H4=>HOCH2CH2O+CH3CHO 2.2E12 0.000 17200 !
! est C2H4+HO2

!
!
!

! NH3 subset

*
!

!
H2Nr+Hr (+M)=H3N (+M)
1.60E+14 0.00 0.00
LOW/ 3.60E+22 -1.76 0.00 /
TROE/ 0.5 1.0E-30 1.0E30 1.0E30 /

! JAM est

!
NH+H2=H2Nr+Hr
2.10E+13 0.00 64.50 !

! M.-K. Bahng and R.G. Macdonald
! Determination of the Rate Constants for the Radical-Radical Reactions
NH2 + NH and NH2 + H2 at 293 K}",
! J. Chem. Phys. A 113 2415-2423 2009

!
H2Nr+Or=HNO+Hr
6.60E+14 -0.50 0.00 !

! J.A. Miller M.D. Smooke R.M. Green R.J. Kee,
! Kinetic modeling of the oxidation of ammonia in flames
! Combust. Sci. Technol. 34, 149-176, 1983

!NH2+O=HNO+H 6.6E13 0.000 0 !

! Inomata S Washida N JPCA 103:5023-5031 1999

! Dransfeld P Hack W Kurzke H Temps F Wagner HGg PCI 20:655 1984

! Adamson JD Farhat SK Morter CL Glass GP Curl RF Philips LF JPC 98:5665
1994

!
H2Nr+Or=NH+HOr
7.00E+12 0.00 0.00 !

DUP
H2Nr+Or=NH+HOr
8.60E-01 4.01 7.00 !
DUP

! Inomata S Washida N JPCA 103:5023-5031 1999
! Dransfeld P Hack W Kurzke H Temps F Wagner HGg PCI 20:655 1984
! Adamson JD Farhat SK Morter CL Glass GP Curl RF Philips LF JPC 98:5665
1994
! Duan X Page M JCP 102:6121-6127 1995
!
H2Nr+HOr=NH+H2O
3.30E+06 1.95 -0.91 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.
! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
!
H2Nr+HO2r=H3N+O2
1.70E+04 1.55 8.48 !

! Sumathi R, Peyerimhoff SD. Chem Phys Lett 1996;263:742-748 (1 atm).
!
H2Nr+HO2r=H2NO+HOr
2.50E+17 -1.28 4.88 !

!NH2+HO2=H2NO+OH 5.0E13 0.000 0 ! ktot
(high pressure limit)
! Sumathi R, Peyerimhoff SD. Chem Phys Lett 1996;263:742-748 (ktot for
nh2+ho2).
!
H2Nr+HO2r=HNO+H2O
1.60E+07 0.55 2.20 !

DUP
H2Nr+HO2r=HNO+H2O
5.70E+15 -1.12 2.96 !

DUP

! Sumathi R, Peyerimhoff SD. Chem Phys Lett 1996;263:742-748.
!
H2Nr+HO2r=HON+H2O
2.10E+07 0.64 3.39 !

! Sumathi R, Peyerimhoff SD. Chem Phys Lett 1996;263:742-748.
!
H2Nr+O2=H2NO+Or
2.60E+11 0.49 121.55 !

! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
!
H2Nr+O2=HNO+HOr
2.90E-02 3.76 76.09 !

! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
!
H2Nr+H2Nr=H3N+NH
5.60E+00 3.53 2.31 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-C Su JV Michael JPCA 113 (2009) 10241-10259.

!

H2Nr+NH=H3N+N

9.60E+03 2.46 0.45 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-C Su JV Michael JPCA 113 (2009) 10241-10259.

!

H2Nr+N=N2+Hr+Hr

7.00E+13 0.00 0.00 !

! Whyte AR Phillips LF CPL 102:451 1983

!

H2Nr+HNO=H3N+NO

5.90E+02 2.95 -14.51 !

! S. Xu, M.C. Lin, Int J Chem Kinet 41: 667-677, 2009

!

H2Nr+NO=N2+H2O

2.60E+19 -2.37 3.64 !

! S. Song R.K. Hanson C.T. Bowman D.M. Golden Int J Chem Kinet 33 715-721, 2001 (kT)

!

H2Nr+NO=NNH+HOr

4.30E+10 0.29 -3.62 !

! S. Song R.K. Hanson C.T. Bowman D.M. Golden Int J Chem Kinet 33 715-721, 2001 (kT)

!

H2Nr+HONO=H3N+NO2

7.10E+01 3.02 -20.67 !

! Mebel AM, Diau EWG, Lin MC, Morokuma K. J Phys Chem 1996;100:7517-7525.

!

H2Nr+NO2=H2NO+NO

8.60E+11 0.11 -4.96 !

! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68.

!

H2Nr+NO2=N2O+H2O

2.20E+11 0.11 -4.96 !

! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68.

!

NH+Hr=N+H2

3.00E+13 0.00 0.00 !

! Davidson DF Kohse-Hoinghaus K Chang AY Hanson RK IJCK 22:513 1990 (reverse)

!

NH+Or=NO+Hr

9.20E+13 0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Frank P Hayman G Just Th Kerr JA Murrells T
Pilling MJ Troe J Walker RW Warnatz J JPCRD 23:847-1033 1994

!
NH+HOr=HNO+Hr

3.20E+14 -0.38 -0.19 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!
NH+HOr=N+H2O

1.60E+07 1.73 -2.41 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!
NH+O2=HNO+Or

2.40E+13 0.00 57.95 ! #r

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Final value used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!NH+O2=HNO+O 4.6E05 2.000 6500 !

! Miller JA, Melius CF. Symp (Int) Combust 1992;24:719-26.

! Preliminary value used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!
NH+O2=NO+HOr

9.90E+10 0.00 6.40 ! #r

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Final value Used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!NH+O2=HNO+O 1.3E06 1.500 100 !

! Miller JA, Melius CF. Symp (Int) Combust 1992;24:719-26.

! Preliminary value used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!
NH+NH=H2Nr+N

5.70E-01 3.88 1.43 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!
NH+N=N2+Hr

3.00E+13 0.00 0.00 !

! JAM est
!

NH+NO=N2O+Hr

2.70E+15 -0.78 0.08 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy
Combust. Sci. 67 (2018) 31-68.

!

NH+NO=N2+HOr
6.80E+14 -0.78 0.08 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy
Combust. Sci. 67 (2018) 31-68.
!

NH+HONO=H2Nr+NO2
1.00E+13 0.00 0.00 !

! JAM est
!

NH+NO2=N2O+HOr
4.10E+12 0.00 0.00 !

! Harrison JA Whyte AR Phillips LF CPL 129:346 1986
!

NH+NO2=HNO+NO
5.90E+12 0.00 0.00 !

! Harrison JA Whyte AR Phillips LF CPL 129:346 1986
!

N+HOr=NO+Hr
3.80E+13 0.00 0.00 !

! Flower WL Hanson RK Kruger CH CST 15:115 1977
! Howard MJ Smith IWM CPL 69:40 1980
!

N+O2=NO+Or
5.90E+09 1.00 26.28 ! #r

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
!

N+NO=N2+Or
9.40E+12 0.14 0.00 !

! M. Abian, M.U. Alzueta, P. Glarborg, Int. J. Chem. Kinet. 47 (2015)
518-532.
!
!

NNH=N2+Hr
1.00E+09 0.00 0.00 !

! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
!

NNH+Hr=N2+H2
1.00E+14 0.00 0.00 !

! JAM est
!

NNH+Or=N2O+Hr
1.90E+14 -0.27 -0.09 !

! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
!

NNH+Or=N2+HOr
 1.20E+13 0.14 -0.91 !
 ! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
 !
 NNH+Or=NH+NO
 5.20E+11 0.38 -1.71 !
 ! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
 !
 NNH+HOr=N2+H2O
 5.00E+13 0.00 0.00 !
 ! JAM est
 !
 NNH+O2=N2+HO2r
 5.60E+14 -0.39 -0.05 !
 ! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.
 !
 NNH+NH=N2+H2Nr
 5.00E+13 0.00 0.00 !
 ! JAM est
 !
 NNH+H2Nr=N2+H3N
 5.00E+13 0.00 0.00 !
 ! JAM est
 !
 NNH+NO=N2+HNO
 5.00E+13 0.00 0.00 !
 ! JAM est
 !
 !
 NH2OH (+M)=H2Nr+HOr (+M)
 1.40E+20 -1.31 268.11 !
 LOW/ 5.40E+37 -5.96 279.42 /
 TROE/ 0.31 1.0E-30 1.0E30 1.0E30 /

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
 C Su JV Michael JPCA 113 (2009) 10241-10259.
 !
 NH2OH+Hr=HNOH+H2
 4.80E+08 1.50 26.15 !
 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 NH2OH+Hr=H2NO+H2
 2.40E+08 1.50 21.20 !
 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 NH2OH+Or=HNOH+HOr
 3.30E+08 1.50 16.17 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

$\text{NH}_2\text{OH} + \text{O} = \text{H}_2\text{NO} + \text{HO}$
1.70E+08 1.50 12.59 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

$\text{NH}_2\text{OH} + \text{HO} = \text{HNOH} + \text{H}_2\text{O}$
1.50E+04 2.61 -14.80 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{HO} = \text{H}_2\text{NO} + \text{H}_2\text{O}$
1.50E+05 2.28 -5.42 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{H}_2\text{N} = \text{HNOH} + \text{H}_3\text{N}$
1.10E-01 4.00 -0.41 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{H}_2\text{N} = \text{H}_2\text{NO} + \text{H}_3\text{N}$
9.50E+00 3.42 -4.24 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{NH} = \text{HNOH} + \text{H}_2\text{N}$
2.90E-03 4.40 6.54 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{NH} = \text{H}_2\text{NO} + \text{H}_2\text{N}$
1.50E-03 4.60 10.14 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.

!

$\text{NH}_2\text{OH} + \text{HO}_2 = \text{HNOH} + \text{H}_2\text{O}_2$
2.90E+04 2.69 39.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

$\text{NH}_2\text{OH} + \text{HO}_2 = \text{H}_2\text{NO} + \text{H}_2\text{O}_2$
1.40E+04 2.69 26.85 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

```

!
H2NO+M=HNO+Hr+M
      2.80E+24  -2.83 271.60      !
      H2O/ 10.0/

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
H2NO+M=HNOH+M
      1.10E+29  -4.00 184.10      !
      H2O/ 10.0/

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
H2NO+Hr=HNO+H2
      3.00E+07   2.00 8.37      !

! JAM est
!
H2NO+Hr=H2Nr+HOr
      5.00E+13   0.00 0.00      !

! JAM est
!
H2NO+Or=HNO+HOr
      3.00E+07   2.00 8.37      !

! JAM est
!
H2NO+HOr=HNO+H2O
      1.00E+14   0.00 0.00      !

! Sun F DeSain JD Scott G Hung PY Thompson RI Glass GP Curl RF JPCA
105:6121-6128 2001
!
H2NO+HO2r=HNO+H2O2
      2.90E+04   2.69 -6.69      !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
H2NO+O2=HNO+HO2r
      2.30E+02   2.99 69.04      !

! See P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog.
Energy Combust. Sci. 67 (2018) 31-68.
!H2NO+O2=HNO+HO2      2.3E02  2.994  18900 !
! Y. Song, H. Hashemi, J.M. Christensen, C. Zou, P. Marshall, P.
Glarborg, Fuel 181 (2016) 358-365.
!
H2NO+H2Nr=HNO+H3N
      3.00E+12   0.00 4.18      !

! JAM est
!
H2NO+NO=HNO+HNO
      2.00E+04   2.00 54.39      !

```


! JAM est

!

H2NO+NO2=HONO+HNO

4.40E+04 2.64 16.90 !

! est as HNO+NO2

!

HNOH+M=HNO+Hr+M

2.00E+24 -2.84 246.58 !
H2O/ 10.0/

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+Hr=H2Nr+HOr

4.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+Hr=HNO+H2

4.80E+08 1.50 1.58 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+Or=HNO+HOr

7.00E+13 0.00 0.00 !

DUP

HNOH+Or=HNO+HOr

3.30E+08 1.50 -1.50 !

DUP

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+HOr=HNO+H2O

2.40E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+HO2r=HNO+H2O2

2.90E+04 2.69 -6.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+HO2r=NH2OH+O2

2.90E+04 2.69 -6.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+O2=HNO+HO2r

3.00E+12 0.00 104.60 !

! JAM est

!

HNOH+H2Nr=H3N+HNO

1.80E+06 1.94 -4.82 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNOH+NO2=HONO+HNO

6.00E+11 0.00 8.37 !

! JAM est

!

!

NO+Hr (+M)=HNO (+M)

1.50E+15 -0.41 0.00 !

LOW/ 2.40E+14 0.21 -6.49 /

TROE/ 0.82 1.0E-30 1.0E30 1.0E30 /

N2/ 1.6/

! Tsang W JPCRD 20:221 1991

! Riley PS Cosic B Fontijn A IJCK 35:374 2003

!

HNO+Hr=NO+H2

6.60E+10 0.94 2.07 !

! MT Nguyen S Zhang J Peeters TN TRuong MT Nguyen Chem Phys Lett 2004 388
94-99

!

HNO+Or=NO+HOr

2.30E+13 0.00 0.00 !

! Inomata S Washida N JPCA 103:5023-5031 1999

!

HNO+HOr=NO+H2O

1.20E+09 1.19 1.40 !

! MT Nguyen S Zhang J Peeters TN TRuong MT Nguyen Chem Phys Lett 2004 388
94-99

!

HNO+HO2r=HNO2+HOr

2.00E+03 2.36 37.57 !

! SH Mousavipour SS Asemani J phys Chem A 2015 119 5553-5565

!

HNO+O2=HO2r+NO

2.00E+13 0.00 66.94 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

HNO+HNO=N2O+H2O

9.00E+08 0.00 12.97 !

! NBS91 Tsang W JPCRD 20:221 1991

!

HNO+NO2=HONO+NO

4.40E+04 2.64 16.90 !

! Mebel AM Lin MC Morokuma K IJCK 30:729-736 1998

!
!

NO+HO2r=NO2+HO2

2.10E+12 0.00 -2.08 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!
!

NO+Or(+M)=NO2(+M)

1.30E+15 -0.75 0.00 !
LOW/ 4.72E+24 -2.87 6.49 /
TROE/ 0.75 1000.0 100000.0 1.0E30 /

! Tsang W JPCRD 20:221 1991

! Allen MT Yetter RA Dryer FL CF 109:449 1997

! Yarwood G Sutherland JW Wickramaaratchi MA Klemm RB JPC 95:8771 1991
(AR)

!

NO2+Hr=NO+HO2

1.30E+14 0.00 1.51 !

! Ko T Fontijn A JPC 95:3984-3987 1991

!

NO2+Or=NO+O2

1.10E+14 -0.52 0.00 !

! Bemand PP Clyne MAA Watson RT JCSFT2 70:564-576 1974

!

NO2+HO2r=HONO+O2

1.90E+00 3.32 12.74 !

! CL Rasmussen J Hansen P Marshall P Glarborg IJCK 40, 454-480 (2008)

!

NO2+HO2r=HNO2+O2

1.90E+01 3.26 20.85 !

! CL Rasmussen J Hansen P Marshall P Glarborg IJCK 40, 454-480 (2008)

!

NO2+NO2=NO+NO+O2

4.50E+12 0.00 115.47 !

! Park J Giles ND Moore J Lin MC JPCA 102:10099 1998

!

NO2+NO2=NO3+NO

9.60E+09 0.73 87.45 !

! Tsang W JPCRD 20:221 1991

!

!

NO+HO2r(+M)=HONO(+M)

1.10E+14 -0.30 0.00 !
LOW/ 3.39E+23 -2.50 0.00 /
TROE/ 0.75 1.0E-30 1.0E30 1.0E30 /

! Fulle D Hamann HF Hippler H Troe J JCP 108:5391 1998

!
 NO2+H2=HONO+Hr
 1.80E+01 3.51 110.04 !
 DUP
 NO2+H2=HONO+Hr
 2.40E+01 3.62 149.79 !
 DUP

 ! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 HONO+Hr=HNO+HOr
 5.60E+10 0.86 20.92 !

 ! Hsu CC Lin MC Mebel AM Melius CF JPCA 101:60 1997
 !
 HONO+Hr=NO+H2O
 8.10E+06 1.89 16.11 !

 ! Hsu CC Lin MC Mebel AM Melius CF JPCA 101:60 1997
 !
 HONO+Or=NO2+HOr
 1.20E+13 0.00 24.94 !

 ! NBS91 Tsang W JPCRD 20:221 1991
 !
 HONO+HOr=NO2+H2O
 1.70E+12 0.00 -2.18 !

 ! Burkholder JB Mellouki A Talukdar R Ravishankara AR IJCK 24:711 1992
 !
 HONO+NO2=HONO2+NO
 2.00E+11 0.00 136.82 !

 ! Park J Giles ND Moore J Lin MC JPCA 102:10099 1998
 !
 HONO+HONO=NO+NO2+H2O
 3.50E-01 3.64 50.79 !

 ! Mebel AM Lin MC Melius CF JPCA 102:1803 1998
 !
 !
 HNO2 (+M)=HONO (+M)
 2.50E+14 0.00 135.14 !
 LOW/ 3.10E+18 0.00 131.80 /
 TROE/ 1.149 1.0E-30 3125.0 1.0E30 /

! CL Rasmussen J Hansen P Marshall P Glarborg IJCK 40, 454-480 (2008)
 !
 NO2+H2=HNO2+Hr
 2.40E+02 3.15 130.12 !

 ! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 HNO2+Or=NO2+HOr
 1.70E+08 1.50 8.37 !

 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000

!
 HNO2+HOr=NO2+H2O
 4.00E+13 0.00 0.00 !

! CL Rasmussen J Hansen P Marshall P Glarborg IJCK 40, 454-480 (2008)
 !
 !

NO2+Or (+M)=NO3 (+M)
 3.50E+12 0.24 0.00 !
 LOW/ 2.50E+20 -1.50 0.00 /
 TROE/ 0.71 1.0E-30 1700.0 1.0E30 /

! Hahn J Luther K Troe J PCCP 2:5098 2000
 !

NO3+Hr=NO2+HOr
 6.00E+13 0.00 0.00 !

! Becker E Rahman MM Schindler RN BBPC 96:776 1992
 !

NO3+Or=NO2+O2
 1.00E+13 0.00 0.00 !

! Atkinson R Baulch DL Cox RA Hampson RF Kerr JA Troe J JPC Ref Data
 1992, 21, 1125-1568.
 !

NO3+HOr=NO2+HO2r
 1.40E+13 0.00 0.00 !

! Atkinson R Baulch DL Cox RA Hampson RF Kerr JA Troe J JPC Ref Data
 1992, 21, 1125-1568.
 !

NO3+HO2r=NO2+O2+HOr
 1.50E+12 0.00 0.00 !

! Becker E Rahman MM Schindler RN BBPC 96:776 1992
 !

NO3+NO2=NO+NO2+O2
 5.00E+10 0.00 12.30 !

! DeMore WB Sander SP Golden DM Molina MJ Hampson RF Kurylo MJ Howard CJ
 Ravishankara AR JPL P 90-1:1 1990
 !
 !

NO2+HOr (+M)=HONO2 (+M)
 3.00E+13 0.00 0.00 !
 LOW/ 2.94E+25 -3.00 0.00 /
 TROE/ 0.4 1.0E-30 1.0E30 1.0E30 /

! Troe J IJCK 33:878 2001
 !

HONO2+Hr=H2+NO3
 5.60E+08 1.50 68.62 !

! Boughton JW Kristyan S Lin MC Chem. Phys 214:219 1997
 !

HONO2+Hr=H2O+NO2
 6.10E+01 3.30 26.30 !

! Boughton JW Kristyan S Lin MC Chem. Phys 214:219 1997

!

HONO2+Hr=HOr+HONO

3.80E+05 2.30 29.19 !

! Boughton JW Kristyan S Lin MC Chem. Phys 214:219 1997

!

HONO2+HOr=H2O+NO3

1.00E+10 0.00 -5.19 !

! Lamb JJ Mozurkewich M Benson SW JPC 88:6441-6448 1984

!

!

N2O(+M)=N2+Or(+M)

9.90E+10 0.00 242.26 !

LOW/ 6.00E+14 0.00 240.35 /

O2/ 1.4/ N2/ 1.7/ H2O/ 12.0/

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker

D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Fc=1.167-1.25E-4T close to 1.0 over 300-2500 K range

! Johnsson JE Glarborg P Dam-Johansen K PCI 24:917 1992 (TBE)

!

N2O+Hr=N2+HOr

6.40E+07 1.83 56.45 !

! SJ Klippenstein LB Harding P Glarborg JA Miller CF 158 (2011) 774-789.

!

N2O+Or=NO+NO

9.20E+13 0.00 115.81 !

! Meagher NE Anderson WR JPCA 104:6013-6031 2000

!

N2O+Or=N2+O2

9.20E+13 0.00 115.81 !

! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy

Combust. Sci. 67 (2018) 31-68.

!

N2O+HOr=N2+HO2r

1.30E-02 4.72 152.97 !

! Mebel AM Diau EWG Lin MC Morokuma K JPC 100:7517-7525 1996

!

N2O+HOr=HNO+NO

1.20E-04 4.33 104.93 !

! Mebel AM Diau EWG Lin MC Morokuma K JPC 100:7517-7525 1996

!

N2O+NO=NO2+N2

5.30E+05 2.23 193.64 !

! Mebel AM Diau EWG Lin MC Morokuma K JPC 100:7517-7525 1996

!

!

!

```

! N2 amine subset
*
!
*****
!
H2Nr+H2Nr=N2H2+H2
      1.70E+08    1.62 49.30 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.
!
H2Nr+H2Nr=H2NN+H2
      7.20E+04    1.88 36.83 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.
!
H2Nr+NH=N2H2+Hr
      4.30E+14   -0.27 -0.32 !

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.
!
HNOH+H2Nr=N2H3+HOr
      1.00E+01    3.46 -1.95 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
HNOH+H2Nr=H2NN+H2O
      8.80E+16   -1.08 4.66 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
H2Nr+H2Nr(+M)=N2H4(+M)
      5.60E+14   -0.41 0.28 !
LOW/  1.60E+34  -5.49 8.31 /
TROE/ 0.31 1.0E-30  1.0E30  1.0E30 /

! SJ Klippenstein LB Harding B Ruscic R Sivaramakrishnan NK Srinivasan M-
C Su JV Michael JPCA 113 (2009) 10241-10259.
!
N2H4=H2NN+H2
      1.40E+14    0.00 313.43    !

! D.-Y. Hwang, A.M. Mebel, J. Phys. Chem. A 2003, 107, 2865-2874
!
N2H4+Hr=N2H3+H2
      7.00E+12    0.00 10.46 !

! Vaghjani GL IJCK 27:777 1995
!N2H4+H=N2H3+H2
      4.5E07    1.800    2613 !
! D.-Y. Hwang, A.M. Mebel, J. Phys. Chem. A 2003, 107, 2865-2874 (factor
7 low at 300 K)
!
N2H4+Hr=H3N+H2Nr
      2.30E+05    1.42 34.32 !

```

! D.-Y. Hwang, A.M. Mebel, J. Phys. Chem. A 2003, 107, 2865-2874 (factor
7 low at 300 K)

!
N2H4+Or=N2H3+HOr
1.50E+11 0.00 -5.31 !

! Vaghjiani GL JPC 104:5479-5489 1996
! Vaghjiani GL JPCA 105:4682-4690 2001

!
N2H4+Or=N2H2+H2O
2.90E+11 0.00 -5.31 !

! Vaghjiani GL JPC 104:5479-5489 1996
! Vaghjiani GL JPCA 105:4682-4690 2001

! Non-OH products assumed
!
N2H4+HOr=N2H3+H2O
1.30E+13 0.00 -1.33 !

! Vaghjiani GL IJCK 33:354-362 2001

!
N2H4+H2Nr=N2H3+H3N
7.60E-01 4.00 16.94 !

! Q.S. Li, X.A.F. Zhang
! Direct dynamics study on the hydrogen abstraction reactions N2H4+R-
>N2H3+RH (R=NH2, CH3)

! J. Chem. Phys. 125 064304 2006
!
N2H4+NO=N2H3+HNO
6.00E+01 3.16 129.06 !

! P. Raghunath and Y.H. Lin and M.C. Lin
! Ab initio chemical kinetics for the N2H4+NOx (x=1-3) reactions and
related reverse processes

! Comp. Theor. Chem. 1046, 73-80, 2014
!
N2H4+NO2=N2H3+HONO
8.20E+01 3.13 37.07 !

! P. Raghunath and Y.H. Lin and M.C. Lin
! Ab initio chemical kinetics for the N2H4+NOx (x=1-3) reactions and
related reverse processes,

! Comp. Theor. Chem. 1046, 73-80, 2014
!
N2H4+NO2=N2H3+HNO2
2.40E-02 4.14 33.25 !

! P. Raghunath and Y.H. Lin and M.C. Lin
! Ab initio chemical kinetics for the N2H4+NOx (x=1-3) reactions and
related reverse processes,

! Comp. Theor. Chem. 1046, 73-80, 2014
!
N2H2+Hr=N2H3
1.30E+14 0.00 16.20 !

! Zheng, JJ Rocha, RJ Pelegrini, M Ferrao, LFA Carvalho, EFV Roberto-
Neto, O Machado, FBC Truhlar, DG
! A product branching ratio controlled by vibrational adiabaticity and
variational effects: Kinetics of the H+trans-N₂H₂ reactions
! J. Chem. Phys. 18 184310 2012
! rough fit to 600-1500 K
!

N₂H₃+Hr=N₂H₂+H₂
2.40E+08 1.50 -0.04 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+Or=N₂H₂+HOr
1.70E+08 1.50 -2.70 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+Or=H₂Nr+HNO
3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+Or=>H₂Nr+NO+Hr
3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+HOr=N₂H₂+H₂O
1.20E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+HOr=H₂NN+H₂O
3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+HOr=H₃N+HNO
1.00E+12 0.00 62.76 !

! JAM est

! N₂H₃+HO₂r=N₂H₂+H₂O₂
1.40E+04 2.69 -6.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! N₂H₃+HO₂r=N₂H₄+O₂
9.20E+05 1.94 8.90 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

N2H3+H2Nr=N2H2+H3N
9.20E+05 1.94 -4.82 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

N2H3+H2Nr=H2NN+H3N
3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

N2H3+NH=N2H2+H2Nr
2.00E+13 0.00 0.00 !

! JAM est

!

!

N2H2+M=NNH+Hr+M
1.90E+27 -3.05 276.59 !
H2O/ 7.0/

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

N2H2+Hr=NNH+H2
1.10E+14 0.00 13.09 !

! Zheng, JJ Rocha, RJ Pelegrini, M Ferrao, LFA Carvalho, EFV Roberto-
Neto, O Machado, FBC Truhlar, DG

! A product branching ratio controlled by vibrational adiabaticity and
variational effects: Kinetics of the H+trans-N2H2 reactions

! J. Chem. Phys. 18 184310 2012

! rough fit to 600-1500 K

!

N2H2+Or=NNH+HOr
3.30E+08 1.50 2.08 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

N2H2+Or=H2Nr+NO
1.00E+13 0.00 0.00 !

! JAM est

!

N2H2+HOr=NNH+H2O
5.90E+01 3.40 5.69 !

! Linder DP Duan X Page M JCP 104:6298 1996

!

N2H2+H2Nr=NNH+H3N
8.80E-02 4.05 6.74 !

! Linder DP Duan X Page M JCP 104:6298 1996

!
 N2H2+NH=NNH+H2Nr
 2.40E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

N2H2+NO=N2O+H2Nr
 4.00E+12 0.00 49.88 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN=NNH+Hr
 3.40E+26 -4.83 193.42 ! 1 ATM

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN=N2+H2
 2.50E+14 0.00 220.85 !

! D.-Y. Hwang, A.M. Mebel, J. Phys. Chem. A 2003, 107, 2865-2874
 !

H2NN=N2H2
 1.30E+14 0.00 196.36 !

! D.-Y. Hwang, A.M. Mebel, J. Phys. Chem. A 2003, 107, 2865-2874
 !

H2NN+Hr=NNH+H2
 4.80E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN+Hr=N2H2+Hr
 7.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN+Or=NNH+HOr
 3.30E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN+Or=H2Nr+NO
 7.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

H2NN+HOr=NNH+H2O
 2.40E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
H2NN+HOr=>H2Nr+NO+Hr
2.00E+12 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
H2NN+HO2r=>H2Nr+NO+HOr
9.00E+12 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
H2NN+HO2r=NNH+H2O2
2.90E+04 2.69 -6.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
H2NN+O2=H2Nr+NO2
1.50E+12 0.00 24.94 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
H2NN+H2Nr=NNH+H3N
1.80E+06 1.94 -4.82 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
!
!

! Cyanide subset

*
!

!
HCN+M=Hr+CN+M
3.40E+35 -5.13 556.47 !
O2/ 1.5/ N2/ 0.0/ H2O/ 10.0/
HCN+N2=Hr+CN+N2
3.60E+26 -2.60 522.54 !

! Tsang W JPCRD 20:221 1991

!
HCN+M=HNC+M
1.60E+26 -3.23 229.70 !
CO2/ 2.0/ H2O/ 7.0/ AR/ 0.7/

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

! P Glarborg P Marshall (mod Ea)
!

CN+H2=HCN+Hr
 1.10E+05 2.60 7.98 !
 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 ! Typo in listing (E=51908) in P. Glarborg, J.A. Miller, B. Ruscic, S.J.
 Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68 !
 !
 HCN+Or=NCO+Hr
 1.40E+04 2.64 20.84 !
 ! Miller JA Bowman CT PECS 15:287 1989
 !
 HCN+Or=NH+CO
 3.50E+03 2.64 20.84 !
 ! Miller JA Bowman CT PECS 15:287 1989
 !
 HCN+Or=CN+HOr
 4.20E+10 0.40 86.46 !
 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 HCN+HOr=CN+H2O
 3.90E+06 1.83 43.10 !
 ! Wooldridge ST Hanson RK Bowman CT IJCK 27:1075-1087 1995
 !
 HCN+HOr=HOCN+Hr
 5.90E+04 2.43 52.30 ! #r
 ! Miller JA Bowman CT PECS 15:287 1989
 !
 HCN+HOr=HNCO+Hr
 2.00E-03 4.00 4.18 !
 ! Miller JA Bowman CT PECS 15:287 1989
 !
 HCN+HOr=H2Nr+CO
 7.80E-04 4.00 16.74 !
 ! Miller JA Bowman CT PECS 15:287 1989
 !
 HCN+O2=CN+HO2r
 3.00E+13 0.00 314.22 !
 ! P Dagaut P Glarborg MU Alzueta PECS 34 (2008) 1-46 est
 !
 HCN+CN=NCCN+Hr
 1.50E+07 1.71 6.40 !
 ! Tsang W JPCRD 21:753-791 1992
 !
 !
 HNC+Hr=HCN+Hr
 7.80E+13 0.00 15.06 !

! Sumathi R Nguyen MT JPCA 102:8013-8020 1998 (fit to reported data)
! Typo in listing (E=0) in P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68 !

!
HNC+Or=NH+CO
4.60E+12 0.00 9.20 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry, Springer 2000

!
HNC+HOr=HNCO+Hr
3.60E+12 0.00 -2.00 !

! Bunkan et al. (2014) !
! Glarborg and Marshall (2016)

!
HNC+HOr=CN+H2O
3.00E+02 3.16 44.35 !

! Bunkan et al. (2014) !
! Glarborg and Marshall (2016)

!
CN+Or=CO+N
1.90E+12 0.46 3.03 !

! Cobos CJ React Kinet Catal Lett 57:43-47 1996

!
CN+HOr=NCO+Hr
1.00E+15 -0.44 0.00 !

! Wooldridge ST Hanson RK Bowman CT IJCK 1996;28:245-58
! Decker, B.K.; Macdonald, R.G. J. Phys. Chem. A 107 9137-9146 2003

!
CN+O2=NCO+Or
5.80E+12 0.00 -1.74 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! Rim KT Hershberger JF JPCA 103:3721-3725 1999

!
CN+O2=NO+CO
1.40E+12 0.00 -1.74 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
! Feng, Wenhui; Hershberger, John F. J Phys Chem A 2009, 113, 3523-3527
(br=20%)

!
CN+NO=NCO+N
9.60E+13 0.00 176.15 !

! Tsang W JPCRD 21:753-791 1992

!
CN+NO2=NCO+NO
5.30E+15 -0.75 1.44 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Park J Hershberger JF JPC 99:3488-3493 1993

!

CN+NO2=CO+N2O

4.90E+14 -0.75 1.44 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Park J Hershberger JF JPC 99:3488-3493 1993

!

CN+NO2=N2+CO2

3.70E+14 -0.75 1.44 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Park J Hershberger JF JPC 99:3488-3493 1993

!

CN+HNO=HCN+NO

1.80E+13 0.00 0.00 !

! Tsang W JPCRD 21:753-791 1992

!

CN+HONO=HCN+NO2

1.20E+13 0.00 0.00 !

! Tsang W JPCRD 21:753-791 1992

!

!CN+N2O=NCN+NO

3.8E03 2.600 3700 ! see

reverse

! Tsang W JPCRD 21:753-791 1992

! Williams BA Papas P Nelson HH JPC 1995;99:13471

!

CN+HNCO=HCN+NCO

3.20E+13 0.00 40.46 !

! C. Sun Y. Liu B. Xu X. Li L. Meng S. Zhang Comp. Theo. Chem. 1014 43-48
2013 (rough fit to data 800-1500 K)

!

CN+HNCO=HNCN+CO

7.70E+13 0.00 39.46 !

! C. Sun Y. Liu B. Xu X. Li L. Meng S. Zhang Comp. Theo. Chem. 1014 43-48
2013 (rough fit to data 800-1500 K)

!

CN+NCO=NCN+CO

1.30E+13 0.00 -1.29 !

! S-Y Tzeng P-H Chen NS Wang LC Lee ZF Xu MC Lin J. Phys. Chem. A 2009,
113, 6314-6325

!

!

HNCO+M=CO+NH+M

1.10E+16 0.00 359.82 !

N2/ 1.5/

! Mertens JD Chang AY Hanson RK Bowman CT IJCK 21:1049 1989

!

HNCO+Hr=H2Nr+CO

3.60E+04 2.49 9.81 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

HNCO+Hr=NCO+H2

9.00E+07 1.66 58.16 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

HNCO+Or=NCO+HOr

2.20E+06 2.11 47.82 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Tsang W JPCRD 21:753-791 1992

!

HNCO+Or=NH+CO2

9.60E+07 1.41 35.65 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

! Tsang W JPCRD 21:753-791 1992

!

HNCO+Or=HNO+CO

1.50E+08 1.57 184.15 !

! He Y Lin MC Wu CK Melius CF PCI 24:711 1992

!

HNCO+HOr=NCO+H2O

3.50E+07 1.50 15.06 !

! Wooldridge ST Hanson RK Bowman CT IJCK 28:361-372 1995

! D Sengupta MT Nguyen J. Chem. Phys. 106 (1997) 9703-9707: NH2+CO2
channel negligible

!

HNCO+HO2r=NCO+H2O2

3.00E+11 0.00 92.05 !

! JAM est

!

HNCO+O2=HNO+CO2

2.00E+13 0.00 246.44 !

! P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Prog. Energy
Combust. Sci. 67 (2018) 31-68.

!

HNCO+H2O=H3N+CO2

2.00E+13 0.00 202.92 !

HNCO+NH=H2Nr+NCO

3.00E+13 0.00 99.16 !

! JAM lr

!

HNCO+HNCO=HNCNH+CO2

6.90E+11 0.00 176.15 !

! He, Y.; Liu, X.; Lin, M.C. Int. J. Chem. Kinet. 23 (1991) 1129-1149
!
!

HOCN+Hr=HNCO+Hr
3.10E+08 0.84 8.02 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HOCN+Hr=H2Nr+CO
1.20E+08 0.61 8.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HOCN+Hr=H2+NCO
2.40E+08 1.50 27.69 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HOCN+Or=HOr+NCO
1.70E+08 1.50 17.29 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HOCN+HOr=H2O+NCO
1.20E+06 2.00 -1.04 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HOCN+H2Nr=NCO+H3N
9.20E+05 1.94 15.25 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
!

HCNO=HCN+Or
4.20E+31 -6.12 256.10 !
PLOG/ 0.1 2.00E+30 -6.03 254.11 /
PLOG/ 1.0 4.20E+31 -6.12 256.10 /
PLOG/ 10.0 5.90E+31 -5.85 259.14 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!

HCNO+Hr=HCN+HOr
7.20E+10 0.84 36.03 !

! Miller JA Klippenstein SJ Glarborg P CF 135:357-362 2003
!

HCNO+Or=HCO+NO
6.30E+13 0.00 0.00 !

! Miller JA Durant JL Glarborg P PCI 1998;27:235-43

!
 HCNO+Or=NCO+HOr
 7.00E+12 0.00 0.00 !

! Miller JA Klippenstein SJ Glarborg P CF 135:357-362 2003
 !

HCNO+HOr=CO+H2NO
 1.00E+13 0.00 -6.23 !

! W Feng JP Meyer JF Hershberger J Phys Chem A 2006, 110, 4458-4464 (63%)
 !

HCNO+HOr=HCO+HNO
 6.00E+12 0.00 -6.23 !

! W Feng JP Meyer JF Hershberger J Phys Chem A 2006, 110, 4458-4464 (37%)
 !

HCNO+CN=HCN+NCO
 6.00E+13 0.00 0.00 !

! Feng WH Hershberger JF JPCA 110:12184 2006
 ! Pang JL Xie HB Zhang SW Ding YH Tang AQ JPCA 112:5251-5257 2008
 !

HCNO+NCO=HCN+NO+CO
 9.60E+12 0.00 0.00 !

! Feng WH Hershberger JF
 ! Kinetics of the NCO + HCNO Reaction
 ! J. Phys. Chem. A, 2007, 111, 3831-3835
 !

NCO+M=N+CO+M
 2.20E+14 0.00 226.15 !
 N2/ 1.5/

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

NCO+Hr=CO+NH
 7.20E+13 0.00 4.18 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

NCO+Or=NO+CO
 2.00E+15 -0.50 0.00 !

! Gao Y MacDonald G JPCA 107:4625-4635 2003
 !

NCO+HOr=HON+CO
 5.30E+12 -0.07 21.45 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !

NCO+HOr=Hr+CO+NO
 8.30E+12 -0.05 75.49 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000

!
 NCO+HO2r=HNCO+O2
 2.00E+13 0.00 0.00 !

! est
 !
 NCO+O2=NO+CO2
 2.00E+12 0.00 83.68 !

! Miller, J. A., and Bowman, C. T., Int. J. Chem. Kinet. 23:289 (1991).
 !
 NCO+NO=N2O+CO
 4.00E+19 -2.19 7.29 !

! Zhu RS Lin MC JPCA 104:10807-10811 2004
 !
 NCO+NO=N2+CO2
 1.50E+21 -2.74 7.63 !

! Zhu RS Lin MC JPCA 104:10807-10811 2004
 !
 NCO+NO2=CO+NO+NO
 2.50E+11 0.00 -2.96 !

! Park J Hershberger JF JPC 99:3488-3493 1993
 ! Wooldridge ST Mertens JD Hanson RK Bowman CT PCI 25:983-991 1994
 !
 NCO+NO2=CO2+N2O
 3.00E+12 0.00 -2.96 !

! Park J Hershberger JF JPC 99:3488-3493 1993
 ! Wooldridge ST Mertens JD Hanson RK Bowman CT PCI 25:983-991 1994
 !
 NCO+HNO=HNCO+NO
 1.80E+13 0.00 0.00 !

! Tsang W JPCRD 21:753-791 1992
 !
 NCO+HONO=HNCO+NO2
 3.60E+12 0.00 0.00 !

! Tsang W JPCRD 21:753-791 1992
 !
 NCO+H3N=HNCO+H2Nr
 2.80E+04 2.48 4.10 !

! Becker K Kurtenbach R Schmidt F Wiesen P BBPC 101:128-133 1997
 !
 NCO+N=N2+CO
 2.00E+13 0.00 0.00 !

! JAM est
 !
 NCO+NCO=CO+CO+N2
 1.80E+13 0.00 0.00 !

! Tsang W JPCRD 21:753-791 1992
 !

```

!
!
*****
****
!   CH3CN subset
*
!
*****
****
!
CH3CN=C2H2Nr+Hr
          7.90E+14   0.00 397.23   !

! K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072
!
CH3CN+Hr=HCN+CH3r
          4.40E+10   0.80 28.45 !

! B Wang H Hou Y Gu JPCA 105 (2001) 156-164
!
CH3CN+Hr=HNC+CH3r
          2.80E+15  -0.32 83.81 !

! B Wang H Hou Y Gu JPCA 105 (2001) 156-164
!
CH3CN+Hr=C2H2Nr+H2
          6.00E+04   3.01 35.66 !

! B Wang H Hou Y Gu JPCA 105 (2001) 156-164
!
CH3CN+Or=CH3r+NCO
          6.00E+09   1.80 34.02 !

! K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072
!
CH3CN+CN=C2H2Nr+HCN
          5.00E+13   0.00 8.37  !

! K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072
!
!
C2H2Nr+Or=CH2O+CN
          1.30E+12   0.64 0.00  !

! K Hoyer mann J Seeba Z Phys Chem 188 (1995) 215-226
!
CH2OH+CN=C2H2Nr+HOr
          5.00E+13   0.00 0.00  !

! JAM est
!
!
!
*****
!   Hydrocarbon-nitrogen subset
*
!
*****

```

!
 CO+NO2=NO+CO2
 9.00E+13 0.00 141.42 !

 ! NBS91 Tsang W JPCRD 20:221 1991
 !
 CO+N2O=N2+CO2
 2.70E+11 0.00 84.67 !

 ! NBS91 Tsang W JPCRD 20:221 1991
 !
 CO2+N=NO+CO
 2.00E+12 0.00 83.68 !

 ! A Fernandez A Goumri A Fontijn JPCA 102 (1998) 168-172
 ! P Glarborg PG Kristensen K Dam-Johansen MU Alzueta A Millera R Bilbao
 EF 14 (2000) 828-838
 !
 CO2+CN=NCO+CO
 3.70E+06 2.16 112.55 !

 ! Wang NS Yang DL Lin MC IJCK 23:151 1991
 !
 HOCO+NO=CO+HONO
 1.50E+12 0.00 0.00 !

 ! Petty JT Harrison JA Moore CB JPC 97:11194 1993
 ! Olkhov RV Li Q Osborne MC Smith IWM PCCP 3:4522-4528 2001
 !
 CH2O+NO2=HONO+HCO
 1.40E-07 5.64 38.58 !

 ! Xu ZF Lin MC IJCK 35:184 2003
 !
 CH2O+NO2=HNO2+HCO
 1.10E-01 4.22 83.05 !

 ! Xu ZF Lin MC IJCK 35:184 2003
 !
 CH2O+CN=HCO+HCN
 1.70E+03 2.72 -5.97 !

 ! Feng WL Wang Y Zhang SW Pang XY CPL 266:43-46 1997
 !
 CH2O+NCO=HNCO+HCO
 6.00E+12 0.00 0.00 !

 ! Tsang W JPCRD 21:753-791 1992
 !
 HCO+NO=HNO+CO
 6.90E+12 0.00 0.00 !

 ! Dammeier J Colberg M Friedrichs G PCCP 9:4177-4188 2007
 !
 HCO+HNO=NO+CH2O
 5.80E-01 3.84 0.48 !

 ! Xu ZF Lin MC IJCK 36:205 2004

!
 HCO+NO2=NO+CO2+Hr
 2.30E+13 0.00 0.00 !

! Dammeier J Colberg M Friedrichs G PCCP 9:4177-4188 2007
 !
 HCO+NO2=HONO+CO
 5.00E+12 0.00 0.00 !

! Dammeier J Colberg M Friedrichs G PCCP 9:4177-4188 2007
 !
 HCO+NO2=NO+CO+HOr
 5.00E+12 0.00 0.00 !

! Dammeier J Colberg M Friedrichs G PCCP 9:4177-4188 2007
 !
 HCO+NCO=HNCO+CO
 3.60E+13 0.00 0.00 !

! Song S Golden DM Hanson RK Bowman CT Senosiain JP Musgrave CB
 Friedrichs G IJCK 35:304-309 2003
 !
 CH4+NO2=CH3r+HONO
 1.10E-01 4.28 110.04 !
 DUP
 CH4+NO2=CH3r+HONO
 7.40E+01 3.42 138.49 !
 DUP

! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 CH4+NO2=CH3r+HNO2
 4.00E-01 4.18 130.54 !

! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 CH4+CN=CH3r+HCN
 8.60E+05 2.30 -0.13 !

! Herbert L Smith IWM Spencer-Smith RD IJCK 24:791-802 1992
 !
 CH4+NCO=CH3r+HNCO
 9.80E+12 0.00 33.97 !

! Schuck A Volpp H-R Wolfrum J CF 99:491 1994
 !
 CH3r+H2Nr=CH4+NH
 2.80E+06 1.94 38.53 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !CH4+NH=CH3+NH2 9.0E13 0.000 20000 ! ROH/WAG94
 !
 CH3r+H2Nr=CH2+H3N
 1.60E+06 1.87 31.67 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000

!
 CH3r+NH=CH3N+Hr
 4.00E+13 0.00 0.00 !

 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 CH3r+NH=N+CH4
 8.20E+05 1.87 24.48 !

 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 CH3r+N=CH2Nr+Hr
 7.10E+13 0.00 0.00 !

 ! Davidson DF Hanson RK PCI 23:267-273 1991
 ! TV Alves, AGS de Oliveira Filho, FR Ornellas, Chemical Physics Letters
 457 (2008) 36-41 (theory)
 !
 CH3r+H2NO=CH3O+H2Nr
 2.00E+13 0.00 0.00 !

 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 CH3r+H2NO=CH4+HNO
 1.60E+06 1.87 12.39 !

 ! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
 Springer 2000
 !
 CH3r+HNO=NO+CH4
 1.50E+11 0.76 1.46 !

 ! YM Choi, MC Lin Int J Chem Kinet 2005 37 261-274
 !
 CH3r+HNO=CH3NO+Hr
 8.10E+03 2.40 25.77 !

 ! YM Choi, MC Lin Int J Chem Kinet 2005 37 261-274
 !
 CH3r+NO=HCN+H2O
 1.50E-01 3.52 16.53 !

 ! JA Miller CF Melius P Glarborg IJCK 30 (1998) 223-228
 !
 CH3r+NO=CH2Nr+HOr
 1.50E-01 3.52 16.53 !

 ! JA Miller CF Melius P Glarborg IJCK 30 (1998) 223-228
 !
 CH3r+NO2=CH3O+NO
 1.10E+13 0.00 0.00 ! !! Cato 19_06

 ! P Glarborg AB Bendtsen JA Miller IJCK 31 (1999) 591-602
 ! Wollenhaupt M Crowley JN JPCA 104:6429-6438 2000
 !

$\text{CH}_3\text{r} + \text{CN} = \text{C}_2\text{H}_2\text{Nr} + \text{Hr}$
 1.00E+14 0.00 0.00 !
 ! JAM est
 !
 $\text{CH}_3\text{r} + \text{HOCN} = \text{CH}_3\text{CN} + \text{HOr}$
 5.00E+12 0.00 8.37 !
 ! JAM est
 !
 $\text{CH}_2 + \text{N}_2 = \text{HCN} + \text{NH}$
 1.00E+13 0.00 309.62 !
 ! JAM est
 !
 $\text{CH}_2 + \text{N} = \text{HCN} + \text{Hr}$
 5.00E+13 0.00 0.00 !
 ! JAM est
 !
 $\text{CH}_2 + \text{NO} = \text{HCNO} + \text{Hr}$
 3.10E+12 0.00 -1.58 !
 ! B Atakan D Kocis J Wolfrum PCI 24:691 1992
 ! Fikri M Meyer S Roggenbuck J Temps F Far Disc 119:223-242 2001
 !
 $\text{CH}_2 + \text{NO} = \text{HCN} + \text{HOr}$
 3.90E+11 0.00 -1.58 !
 ! B Atakan D Kocis J Wolfrum PCI 24:691 1992
 ! Fikri M Meyer S Roggenbuck J Temps F Far Disc 119:223-242 2001
 !
 $\text{CH}_2 + \text{NO}_2 = \text{CH}_2\text{O} + \text{NO}$
 5.90E+13 0.00 0.00 !
 ! Seidler V Temps F Wagner HGg Wolf M JPC 93:1070 1989
 !
 $\text{CH}_2(\text{S}) + \text{H}_3\text{N} = \text{CH}_4\text{Nr} + \text{Hr}$
 3.00E+13 0.00 0.00 !
 ! est
 !
 $\text{CH}_2(\text{S}) + \text{NO} = \text{HCN} + \text{HOr}$
 2.00E+13 0.00 0.00 !
 ! JAM est
 !
 $\text{CH}_2(\text{S}) + \text{NO} = \text{CH}_2 + \text{NO}$
 1.00E+14 0.00 0.00 !
 ! Baulch DL Cobos CJ Cox RA Frank P Hayman G Just Th Kerr JA Murrells T
 Pilling MJ Troe J Walker RW Warnatz J JPCRD 23:847-1033 1994
 !
 $\text{CH}_2(\text{S}) + \text{N}_2\text{O} = \text{CH}_2\text{O} + \text{N}_2$
 3.80E+13 0.00 0.00 !
 ! M Koch, F Temps, R Wagener, HG Wagner,

! "Kinetics of the reactions of CH₂ (̃1A₁) with CH₃C₂H, HCN, CO₂, N₂O and COS."

! Ber Bunsenges phys Chem 94 (1990) 645-650.

!

CH+N₂=Hr+NCN

	2.50E+09	0.89	69.54	!	1 atm
PLOG/ 0.01	5.90E+08	1.06	66.78	/	
PLOG/ 0.03	5.90E+08	1.06	66.73	/	
PLOG/ 0.1	6.20E+08	1.05	66.78	/	
PLOG/ 0.3	9.00E+08	1.01	67.45	/	
PLOG/ 1.0	2.50E+09	0.89	69.54	/	
PLOG/ 3.0	9.20E+09	0.75	72.84	/	
PLOG/ 10.0	3.00E+10	0.62	77.32	/	
PLOG/ 30.0	3.80E+10	0.62	81.42	/	
PLOG/ 100.0	9.50E+09	0.81	85.10	/	

!H+NCN=CH+N₂ 7.6E15 -0.680 297 ! 1 atm

! PLOG/1.000E-02 1.8E15 -0.510 -368/

! fit btw. 500 and 2500 K with MAE of 2.0%, 4.1%

! PLOG/3.000E-02 1.8E15 -0.510 -374/

! fit btw. 500 and 2500 K with MAE of 2.0%, 4.1%

! PLOG/1.000E-01 1.9E15 -0.520 -361/

! fit btw. 500 and 2500 K with MAE of 2.1%, 4.2%

! PLOG/3.000E-01 2.7E15 -0.560 -209/

! fit btw. 500 and 2500 K with MAE of 2.2%, 4.3%

! PLOG/1.000E00 7.6E15 -0.680 297/

! fit btw. 500 and 2500 K with MAE of 2.2%, 4.5%

! PLOG/3.000E00 2.8E16 -0.830 1082/

! fit btw. 500 and 2500 K with MAE of 2.0%, 4.4%

! PLOG/1.000E01 9.0E16 -0.950 2151/

! fit btw. 500 and 2500 K with MAE of 1.4%, 3.5%

! PLOG/3.000E01 1.1E17 -0.960 3138/

! fit btw. 500 and 2500 K with MAE of 0.9%, 1.8%

! PLOG/1.000E02 2.9E16 -0.760 4013/

! fit btw. 500 and 2500 K with MAE of 1.9%, 5.4%

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure", Combust. Flame, submitted (2017).

! Final value used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.

Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!CH+N₂=H+NCN 5.3E09 0.79 16770 ! 1 atm

! Preliminary value used in P. Glarborg, J.A. Miller, B. Ruscic, S.J.

Klippenstein, Prog. Energy Combust. Sci. 67 (2018) 31-68

!

CH+N₂=HNCN

	1.40E+23	-3.74	66.19	!	1 atm
PLOG/ 0.01	6.00E+23	-4.41	60.29	/	
PLOG/ 0.03	7.30E+23	-4.30	61.76	/	
PLOG/ 0.1	7.30E+23	-4.17	63.60	/	
PLOG/ 0.3	4.80E+23	-4.00	65.14	/	
PLOG/ 1.0	1.40E+23	-3.74	66.19	/	
PLOG/ 3.0	1.70E+22	-3.38	66.27	/	
PLOG/ 10.0	6.80E+20	-2.90	65.65	/	
PLOG/ 30.0	1.80E+19	-2.37	64.56	/	
PLOG/ 100.0	3.10E+17	-1.78	63.76	/	

!HNCN=CH+N₂ 1.5E30 -5.380 83030 ! 1 atm

! PLOG/1.000E-02 5.9E30 -6.040 81600/
 ! fit btw. 500 and 2500 K with MAE of 3.3%, 7.1%
 ! PLOG/3.000E-02 7.3E30 -5.940 81960/
 ! fit btw. 500 and 2500 K with MAE of 3.5%, 7.7%
 ! PLOG/1.000E-01 7.4E30 -5.800 82400/
 ! fit btw. 500 and 2500 K with MAE of 3.9%, 8.6%
 ! PLOG/3.000E-01 4.9E30 -5.640 82770/
 ! fit btw. 500 and 2500 K with MAE of 4.4%, 9.7%
 ! PLOG/1.000E00 1.5E30 -5.380 83030/
 ! fit btw. 500 and 2500 K with MAE of 5.1%, 11.1%
 ! PLOG/3.000E00 1.8E29 -5.030 83060/
 ! fit btw. 500 and 2500 K with MAE of 5.7%, 12.4%
 ! PLOG/1.000E01 7.6E27 -4.540 82910/
 ! fit btw. 500 and 2500 K with MAE of 6.6%, 13.8%
 ! PLOG/3.000E01 2.0E26 -4.010 82650/
 ! fit btw. 500 and 2500 K with MAE of 7.0%, 14.4%
 ! PLOG/1.000E02 3.7E24 -3.430 82470/
 ! fit btw. 500 and 2500 K with MAE of 7.4%, 14.7%
 ! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and
 Modeling of Relevance to Prompt-NO Formation at High Pressure",
 ! Combust. Flame, submitted (2017).
 !
 CH+H3N=CH2Nr+Hr+Hr
 4.40E+13 0.00 -2.64 !

 ! Becker KH Engelhardt B Geiger H Kurtenbach R Wiesen P CPL 210:135-140
 1993
 !
 CH+N=CN+Hr
 1.30E+13 0.00 0.00 !

 ! Messing I Filseth SV Sadowski CM Carrington T JCP 74:3874 1981
 !
 CH+NO=CO+NH
 9.10E+12 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH+NO=NCO+Hr
 1.80E+13 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH+NO=HCN+Or
 7.90E+13 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !
 CH+NO=CN+HOr
 1.10E+12 0.00 0.00 !

 ! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
 D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005
 !

CH+NO=HCO+N

6.80E+12 0.00 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH+NO₂=HCO+NO

1.00E+14 0.00 0.00 !

! Wagal SS Carrington T Filseth SV Sadowski CM CP 69:61 1982

! Rim KT Hershberger F JPCA 102:5898 1998

!

CN+N=C+N₂

5.90E+14 -0.40 0.00 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker
D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

!

CH+N₂O=HCN+NO

1.90E+13 0.00 -2.14 !

! Becker KH Engelhardt B Geiger H Kurtenbach R Wiesen P CPL 210:135-140
1993

!

C+NO=CN+Or

2.00E+13 0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Frank P Hayman G Just Th Kerr JA Murrells T
Pilling MJ Troe J Walker RW Warnatz J JPCRD 23:847-1033 1994

!

C+NO=CO+N

2.80E+13 0.00 0.00 !

! Baulch DL Cobos CJ Cox RA Frank P Hayman G Just Th Kerr JA Murrells T
Pilling MJ Troe J Walker RW Warnatz J JPCRD 23:847-1033 1994

!

C+N₂O=CN+NO

4.80E+12 0.00 0.00 !

! Dorthe G Caubet P Vias Th Barrere B Marchais J JPC 95:5109-5116 1991

!

CH₃OH+NO₂=HONO+CH₂OH

1.50E+02 3.32 83.83 !

! Xiao C-X Yan N Zou M Hou S-C Kou Y Liu W Zhang S J Mol Cat A Chem
252:202-211 2006

!

CH₃OH+NO₂=HNO₂+CH₂OH

2.40E+03 2.90 114.93 !

! Xiao C-X Yan N Zou M Hou S-C Kou Y Liu W Zhang S J Mol Cat A Chem
252:202-211 2006

!

CH₃O+HNO=NO+CH₃OH

3.20E+13 0.00 0.00 !

! He Y Sanders WA Lin MC JPC 92:5474 1988

!

CH3O+NO=HNO+CH2O
 7.50E+12 0.00 8.44 !
 DUP
 CH3O+NO=HNO+CH2O
 2.50E+18 -2.56 0.00 !
 DUP

 ! Caralp F Rayez M-T Forst W Gomez N Delcroix B Fittschen C Devolder P
 JCSFT 94:3321-3330 1998
 !
 CH3O+NO2=HONO+CH2O
 6.00E+12 0.00 9.56 !

 ! McCaulley JA Anderson SM Jeffries JB CP Lett. 115:180 1985
 !
 CH2OH+HNO=NO+CH3OH
 3.00E+13 0.00 0.00 !

 ! CL Rasmussen AE Rasmussen P Glarborg CF 154 (2008) 529-545 est
 !
 CH2OH+NO=HNCO+H2O
 1.00E+11 0.00 0.00 !

 ! Nesbitt FL Payne WA Stiff LJ JPC 93:5158 1989 (ktot=1.3E12)
 ! W. Feng, E. Janssen, J. F. Hershberger, J. Phys. Chem. A 2016, 120,
 1145-1152 (10% HNCO+H2O; 90% adduct; low pressure)
 !
 CH2OH+NO2=HONO+CH2O
 5.00E+12 0.00 0.00 !

 ! Nesbitt FL Payne WA Stiff LJ JPC 93:5158 1989
 !
 CH3OO+NO=CH3O+NO2
 1.40E+12 0.00 -2.99 !

 ! Mebel AM Lin MC JPCA 103:2088-2096 1999
 !
 C2H6+NO2=C2H5r+HONO
 3.30E+00 3.84 100.00 !
 DUP
 C2H6+NO2=C2H5r+HONO
 8.50E+01 3.45 133.89 !
 DUP

 ! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 C2H6+NO2=C2H5r+HNO2
 3.20E+02 3.19 110.88 !

 ! J. Chai, CF Goldsmith Proc Combust Inst 36 2017 617-626
 !
 C2H6+CN=C2H5r+HCN
 1.20E+08 1.80 -4.16 !

 ! Herbert L Smith IWM Spencer-Smith RD IJCK 24:791-802 1992
 !
 C2H6+NCO=C2H5r+HNCO
 1.50E-09 6.89 -12.18 !

! Schuck A Volpp H-R Wolfrum J CF 99:491 1994
!
C2H5r+N=C2H4_Olef+NH
4.30E+13 0.00 0.00 !

! Stief LJ Nesbitt FL Payne WA Kuo SC Tao W Klemm RB JCP 102:5309-5316
1995
!
C2H5r+N=CH3r+CH2Nr
2.30E+13 0.00 0.00 !

! Stief LJ Nesbitt FL Payne WA Kuo SC Tao W Klemm RB JCP 102:5309-5316
1995
!
!C2H5r+NO2=CH3CH2O+NO
4.00E+13 -0.20 0.00 ! !!4.00E+13 -0.20 0.00 Cato 19/06

! Hennig G Wagner HGg BBPC 99:989-994 1995 (p)
!
!C2H4+CN=CH2CHCN+H 5.9E14 -0.240 0 !
! Herbert L Smith IWM Spencer-Smith RD IJCK 24:791-802 1992
!
!C2H4+NCO=adduct !
! Becker KH Kurtenbach R Wiesen P JPC 99:5986-5991 1995
!
C2H3r_Olef+NO=HCN+CH2O
7.00E+21 -3.38 4.29 !

! Stribel F Jusinski LE Fahr A Halpern JB Klippenstein SJ Taatjes CA PCCP
6:2216-2223 2004
!
C2H3r_Olef+HONO=C2H4_Olef+NO2
8.10E+05 1.87 23.03 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg PCI 33
(2011) 449-457.
! est CH3+HONO
!
C2H3r_Olef+HNO2=C2H4_Olef+NO2
8.10E+05 1.87 20.24 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg PCI 33
(2011) 449-457.
! est CH3+HNO2
!
C2H3r_Olef+NO2=CH2CHO+NO
7.70E+14 -0.60 0.00 !

! WD Geppert AJ Eskola RB Timonen L Halonen JPCA 108 (2004) 4232-4238
!
!C2H2+NH2=NH2C2H2 4.6E06 8.310 7430 !
! Moskaleva LV Lin MC JPCA 102:4687-4693 1998 (0.46 bar)
!
!C2H2+CN=C2HCN+H 3.6E15 -0.530 0 !
! Herbert L Smith IWM Spencer-Smith RD IJCK 24:791-802 1992
!

$C_2H_2 + NCO = HCCO + HCN$
 1.40E+12 0.00 7.59 !
 ! Becker KH Kurtenbach R Wiesen P JPC 99:5986-5991 ($C_2H_4 + NCO$) 1995
 !
 $C_2H + H_3N = C_2H_2 + H_2N$
 7.20E+12 0.00 -3.08 !
 ! Carl SA Elsamra RMI Kulkami RM Nguyen HMT Peeters J JPCA 108:3695-3698
 2004
 !
 $C_2H + NO = HCN + CO$
 4.60E+13 0.00 2.38 !
 ! Peeters J van Look H Ceursters B JPCA 100:15124-15129 1996 (ktot)
 ! W Feng JF Hersberger J. Phys. Chem. A 2013, 117, 3585-3592 (pr)
 !
 $C_2H + NO = CN + HCO$
 1.40E+13 0.00 2.38 !
 ! Peeters J van Look H Ceursters B JPCA 100:15124-15129 1996 (ktot)
 ! W Feng JF Hersberger J. Phys. Chem. A 2013, 117, 3585-3592 (pr)
 !
 $C_2H + NO_2 = HCCO + NO$
 4.60E+13 0.00 -1.08 !
 ! Carl, S.A.; Nguyen, H.M.T.; Nguyen, M.T.; Peeters, J. J. Chem. Phys.
 118, 10996-11008, 2003 (ktot)
 !
 $C_2 + N_2 = CN + CN$
 1.50E+13 0.00 174.60 !
 ! Sommer T Kruse T Roth P Hippler H JPCA 101, 3720-3725 1997
 !
 $C_2 + NO = C_2O + N$
 2.30E+13 0.00 36.15 !
 ! Kruse T Roth P IJCK 31:11-21 1999
 !
 $CH_3CH_2O + NO = CH_3CHO + HNO$
 6.60E+12 0.00 0.00 !
 ! Daële V Ray A Vassalli I Poulet G Le Bras G IJCK 27:1121-1133 1995
 !
 $CH_3CH_2O + NO_2 = CH_3CHO + HONO$
 1.70E+12 0.00 0.00 !
 ! Batt L Int. Rev. Phys. Chem. 6:53-90 1987
 ! Frost MJ Smith IWM JCSFT 86:1751-1756 1990
 !
 $CH_2CH_2OH + NO_2 = CH_2O + CH_2OH + NO$
 7.00E+12 0.00 0.00 !
 ! Doughty A Barnes FJ Bromly JH Haynes BS PCI 26 1996 ($p = HOCH_2CH_2O + NO$)
 !
 $CH_2CHO + NO = HCN + HOCHO$
 7.00E+21 -3.38 4.29 !

! est as C2H3+NO
!
CH2CHO+NO2=CH2CO+HONO
2.00E+15 -0.68 5.98 !

! Doughty A Barnes FJ Bromly JH Haynes BS PCI 26 1996
!
CH3CO+NO2=>CH3r+CO2+NO
1.50E+13 0.00 0.00 !

! Slagle IR Gutman D J Am Chem Soc 104, 4741, 1982 (p=CH3CO2+NO)
!
HCCO+N=HCN+CO
5.00E+13 0.00 0.00 !

! JAM est
!
HCCO+NO=HCNO+CO
7.50E+12 0.00 -2.83 !

! JP Meyer JF Hershberger J Phys Chem B 2005, 109, 8363 (78%)
! Carl, S.A.; Sun, Q.; Vereecken, L.; Peeters, J. J. Phys. Chem. A 2002
106 12242-12247
!
HCCO+NO=HCN+CO2
2.10E+12 0.00 -2.83 !

! JP Meyer JF Hershberger J Phys Chem B 2005, 109, 8363 (22%)
! Carl, S.A.; Sun, Q.; Vereecken, L.; Peeters, J. J. Phys. Chem. A 2002
106 12242-12247
!
HCCO+NO2=HCNO+CO2
1.60E+13 0.00 0.00 !

! Temps F Wagner HGg Wolf M ZPC (Munich) 176:27 1992 (p)
!
C2O+NO=CO+NCO
1.00E+14 0.00 2.80 !

! Thweat WD Erickson MA Hershberger JF JPCA 108:74-79 2004 (p)
!
C2O+NO2=CO2+NCO
5.10E+13 0.00 0.52 !

! Thweat WD Erickson MA Hershberger JF JPCA 108:74-79 2004 (p)
!
!
NCN+M=C+N2+M
8.90E+14 0.00 259.83 ! 966-1900 K

! J Dammeier, N Fassheber, G Friedrichs, Phys. Chem. Chem. Phys., 2012,
14, 1030-1037
! A Busch, N. Gonzalez-Garcia, G. Lendvay, M. Olzmann J. Phys. Chem. A
2015, 119, 7838-7846
! (4.2E14 / 0 / 57870 (1790-2960 K) good agreement in overlap
!
Hr+NCN=HNCN
1.50E+30 -5.43 18.47 ! 1 atm

PLOG/ 0.01 3.90E+23 -4.34 22.37 /
 PLOG/ 0.03 3.30E+25 -4.71 17.16 /
 PLOG/ 0.1 5.60E+27 -5.13 15.65 /
 PLOG/ 0.3 1.70E+29 -5.36 16.51 /
 PLOG/ 1.0 1.50E+30 -5.43 18.47 /
 PLOG/ 3.0 2.60E+30 -5.34 20.38 /
 PLOG/ 10.0 1.20E+30 -5.09 22.07 /
 PLOG/ 30.0 1.90E+29 -4.72 22.91 /
 PLOG/ 100.0 5.10E+27 -4.15 22.47 /

!HNCN=H+NCN 1.97E28 -4.23
 88920.0

! PLOG/1.000E-02 1.3E24 -4.400 88870/
 ! fit btw. 500 and 2500 K with MAE of 4.2%, 9.1%
 ! PLOG/3.000E-02 1.1E26 -4.770 87620/
 ! fit btw. 500 and 2500 K with MAE of 3.7%, 7.6%
 ! PLOG/1.000E-01 1.9E28 -5.200 87270/
 ! fit btw. 500 and 2500 K with MAE of 3.3%, 7.0%
 ! PLOG/3.000E-01 5.9E29 -5.430 87470/
 ! fit btw. 500 and 2500 K with MAE of 3.2%, 7.0%
 ! PLOG/1.000E00 5.2E30 -5.500 87950/
 ! fit btw. 500 and 2500 K with MAE of 3.4%, 7.4%
 ! PLOG/3.000E00 9.3E30 -5.410 88410/
 ! fit btw. 500 and 2500 K with MAE of 3.8%, 8.2%
 ! PLOG/1.000E01 5.1E30 -5.180 88850/
 ! fit btw. 500 and 2500 K with MAE of 4.4%, 9.6%
 ! PLOG/3.000E01 6.9E29 -4.800 89020/
 ! fit btw. 500 and 2500 K with MAE of 5.2%, 11.1%
 ! PLOG/1.000E02 2.0E28 -4.230 88920/
 ! fit btw. 500 and 2500 K with MAE of 6.2%, 13.1%

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
 ! Combust. Flame, submitted (2017).

!

NCN+Hr=HCN+N

2.20E+11 0.71 22.26 ! 1 atm
 PLOG/ 0.01 2.20E+11 0.71 22.26 /
 PLOG/ 0.03 2.20E+11 0.71 22.26 /
 PLOG/ 0.1 2.20E+11 0.71 22.26 /
 PLOG/ 0.3 2.20E+11 0.71 22.26 /
 PLOG/ 1.0 2.20E+11 0.71 22.26 /
 PLOG/ 3.0 2.20E+11 0.71 22.26 /
 PLOG/ 10.0 2.20E+11 0.71 22.27 /
 PLOG/ 30.0 2.30E+11 0.70 22.29 /
 PLOG/ 100.0 2.50E+11 0.69 22.47 /

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
 ! Combust. Flame, submitted (2017).

!

NCN+Hr=HNC+N

4.30E-04 4.69 10.18 ! 1 atm
 PLOG/ 0.01 3.90E-04 4.70 10.21 /
 PLOG/ 0.03 3.90E-04 4.70 10.21 /
 PLOG/ 0.1 4.00E-04 4.70 10.21 /
 PLOG/ 0.3 4.00E-04 4.70 10.20 /
 PLOG/ 1.0 4.30E-04 4.69 10.18 /
 PLOG/ 3.0 4.90E-04 4.67 10.14 /

PLOG/ 10.0 7.10E-04 4.62 10.08 /
PLOG/ 30.0 1.70E-03 4.52 10.97 /
PLOG/ 100.0 9.60E-03 4.32 15.23 /

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).

!

NCN+Or=CN+NO

2.50E+13 0.17 -0.14 !

! R. S. Zhu and M. C. Lin, J. Phys. Chem. A 2007, 111, 6766-6771

!

NCN+HOr=NCNOH

1.80E+32 -6.37 16.42 ! 1 atm
PLOG/ 0.01 1.60E+31 -6.65 11.37 /
PLOG/ 0.03 2.90E+31 -6.59 12.30 /
PLOG/ 0.05 3.80E+31 -6.55 12.73 /
PLOG/ 0.1 2.20E+32 -6.70 14.31 /
PLOG/ 0.3 1.60E+32 -6.51 14.97 /
PLOG/ 1.0 1.80E+32 -6.37 16.42 /
PLOG/ 3.0 5.40E+31 -6.08 17.18 /
PLOG/ 10.0 6.50E+30 -5.67 17.64 /
PLOG/ 30.0 2.20E+29 -5.11 17.10 /
PLOG/ 100.0 1.50E+27 -4.35 15.44 /

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).

!

NCN+HOr=NCO+NH

1.70E+18 -1.83 17.33 ! 1 atm
PLOG/ 0.01 8.60E+14 -0.95 3.07 /
PLOG/ 0.03 2.60E+15 -1.08 4.72 /
PLOG/ 0.05 5.40E+15 -1.17 5.82 /
PLOG/ 0.1 1.70E+16 -1.30 7.71 /
PLOG/ 0.3 1.40E+17 -1.55 11.68 /
PLOG/ 1.0 1.70E+18 -1.83 17.33 /
PLOG/ 3.0 1.00E+19 -2.03 23.46 /
PLOG/ 10.0 2.20E+19 -2.08 30.71 /
PLOG/ 30.0 6.40E+18 -1.88 37.10 /
PLOG/ 100.0 6.30E+16 -1.25 42.76 /

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).

!

NCN+HOr=HCN+NO

2.60E+08 1.22 15.03 ! 1 atm
PLOG/ 0.01 2.90E+05 2.04 6.30 /
PLOG/ 0.03 6.90E+05 1.94 7.31 /
PLOG/ 0.05 1.20E+06 1.87 7.96 /
PLOG/ 0.1 2.90E+06 1.76 9.05 /
PLOG/ 0.3 1.90E+07 1.54 11.41 /
PLOG/ 1.0 2.60E+08 1.22 15.03 /
PLOG/ 3.0 4.10E+09 0.89 19.35 /
PLOG/ 10.0 7.10E+10 0.56 25.04 /
PLOG/ 30.0 3.90E+11 0.38 30.66 /

PLOG/ 100.0 2.60E+11 0.48 36.21 /

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).du

!
NCN+O2=NCO+NO
1.30E+12 0.00 96.93 !

! N Fasseber, G Friedrichs, Int. J. Chem. Kinet. 47 586-595, 2015

!
NCN+NO=CN+N2O
1.90E+12 0.00 26.28 ! 704-1659 K

! J Dammeier, G Friedrichs, J. Phys. Chem. A 2011, 115, 14382-14390
! low T recombination (O Welz M Olzmann J. Phys. Chem. A 2012, 116, 7293-7301)

!
!NCN+NO2=NCNO+NO 1.2E-11 0.000 5463*R !
! T-J Yang NS Wang LC Lee ZF Xu MC Lin J. Phys. Chem. A 2008, 112, 10185-10192

!
NCN+NCN=CN+CN+N2
3.70E+12 0.00 0.00 ! 966-1900 K

! J Dammeier, N Fasseber, G Friedrichs, Phys. Chem. Chem. Phys., 2012, 14, 1030-1037

!
NCN+H2=HNCN+Hr
4.10E+13 0.00 100.83 !

! N Fasseber N Lamoureux, G Friedrichs, Phys. Chem. Chem. Phys.

!
HNCN+Or=HNC+NO
1.20E+14 -0.05 0.30 !

! S. Xu and M. C. Lin, Proc. Combust. Inst. 2009, 32, 99-106.

!
HNCN+Or=NH+NCO
5.60E+13 -0.05 0.30 !

! S. Xu and M. C. Lin, Proc. Combust. Inst. 2009, 32, 99-106.

!
HNCN+Or=CN+HNO
9.40E+12 -0.05 0.30 !

! S. Xu and M. C. Lin, Proc. Combust. Inst. 2009, 32, 99-106.

!
HNCN+HOr=NCN+H2O
1.00E+05 2.48 -7.90 !

! S. Xu and M. C. Lin, J. Phys. Chem. A, 2007, 111, 6730-6740.

!
HNCN+O2=NCN+HO2r
1.30E+08 1.28 101.25 !

! S. Xu and M. C. Lin, Proc. Combust. Inst. 2009, 32, 99-106.

!

NCNOH=NCO+NH

	5.80E+36	-7.62	249.53	!	1 atm
PLOG/ 0.01	2.10E+35	-7.73	236.06	/	
PLOG/ 0.03	4.00E+35	-7.67	237.94	/	
PLOG/ 0.05	4.00E+35	-7.61	238.82	/	
PLOG/ 0.1	8.50E+36	-7.93	242.38	/	
PLOG/ 0.3	8.60E+34	-7.20	242.25	/	
PLOG/ 1.0	5.80E+36	-7.62	249.53	/	
PLOG/ 3.0	1.00E+36	-7.27	253.30	/	
PLOG/ 10.0	7.10E+34	-6.81	257.90	/	
PLOG/ 30.0	6.20E+32	-6.10	261.08	/	
PLOG/ 100.0	1.90E+29	-4.97	262.96	/	

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).
!

NCNOH=>NCNO+Hr

	2.10E+10	-1.12	279.66	!	1 atm; made irreversible!
PLOG/ 0.01	9.90E-28	8.75	212.05	/	
PLOG/ 0.03	1.50E+03	0.49	300.29	/	
PLOG/ 0.05	1.60E-16	5.85	238.32	/	
PLOG/ 0.1	1.60E-04	2.58	268.45	/	
PLOG/ 0.3	9.30E-01	1.66	268.57	/	
PLOG/ 1.0	2.10E+10	-1.12	279.66	/	
PLOG/ 3.0	1.50E+15	-2.31	280.58	/	
PLOG/ 10.0	5.90E+20	-3.63	286.23	/	
PLOG/ 30.0	1.70E+24	-4.35	289.28	/	
PLOG/ 100.0	9.20E+26	-4.81	292.71	/	

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).
!

NCNOH=HCN+NO

	4.20E+30	-6.14	247.94	!	1 atm
PLOG/ 0.01	1.50E+23	-4.81	219.95	/	
PLOG/ 0.03	1.20E+24	-4.88	225.14	/	
PLOG/ 0.05	5.40E+24	-4.97	227.99	/	
PLOG/ 0.1	1.20E+27	-5.53	234.14	/	
PLOG/ 0.3	1.70E+27	-5.35	238.32	/	
PLOG/ 1.0	4.20E+30	-6.14	247.94	/	
PLOG/ 3.0	2.10E+31	-6.14	252.96	/	
PLOG/ 10.0	3.40E+31	-5.99	257.94	/	
PLOG/ 30.0	5.30E+30	-5.57	261.33	/	
PLOG/ 100.0	4.30E+28	-4.78	263.38	/	

! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).
!

NCNOH+Hr=HNCN+HOr

1.20E+14	0.00	0.00	!
----------	------	------	---

!NCNOH+H=NH+CNOH

6.0E13	0.000	0	!
--------	-------	---	---

NCNOH+Or=>NCNO+HOr

1.20E+14	0.00	0.00	!	made irreversible!
----------	------	------	---	--------------------

```

!NCNOH+O=NO+CNOH          6.0E13  0.000  0 !
NCNOH+Or=CN+HONO
    6.00E+13  0.00 0.00 !
NCNOH+HOr=>NCNO+H2O
    6.00E+13  0.00 0.00 ! made irreversible!
NCNO+Hr=>HNC+NO
    6.00E+13  0.00 0.00 ! made irreversible!
NCNO+Or=>NCO+NO
    6.00E+13  0.00 0.00 ! made irreversible!

!NCNO+OH=>NOCN+NO          6.0E13  0.000  0 ! made
irreversible!
! S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, "Theory and
Modeling of Relevance to Prompt-NO Formation at High Pressure",
! Combust. Flame, submitted (2017).
! rough estimates
!
HNCNH+Hr=HNCN+H2
    4.80E+08  1.50 30.64 !

! est 2x ch2nh+h
!
HNCNH+Or=HNCN+HOr
    3.40E+08  1.50 19.37 !

! est 2x ch2nh+o
!
HNCNH+HOr=HNCN+H2O
    2.40E+06  2.00 -0.37 !

! est 2x ch2nh+oh
!
!
!
*****
! Nitro and nitroso hydrocarbon subset
*
!
*****
!
!
CH3r+NO (+M)=CH3NO (+M)
    9.00E+12  0.00 0.80 !
    LOW/  2.50E+16  0.00 -11.89 /
    TROE/  5.0  1.0E-30  120.0 1.0E30 /

! Davies JW Green NJB Pilling MJ JCSFT 87:2317-2324 1991
!
CH3NO+Hr=CH2NO+H2
    4.40E+08  1.50 1.58 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000
!
CH3NO+Or=CH2NO+HOr
    3.30E+08  1.50 15.13 !

```

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3NO+HOr=CH2NO+H2O
3.60E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3NO+CH3r=CH2NO+CH4
7.90E+05 1.87 22.66 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3NO+H2Nr=CH2NO+H3N
2.80E+06 1.94 4.49 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
!CH3NO+H=CH3+HNO ! see
reverse

!
CH3NO+Or=CH3r+NO2
1.70E+06 2.08 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3NO+HOr=CH3r+HONO
2.50E+12 0.00 4.16 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH2NO=HNCO+Hr
2.30E+42 -9.11 225.26 ! 1 atm
PLOG/ 0.1 6.90E+41 -9.30 216.32 /
PLOG/ 1.0 2.30E+42 -9.11 225.26 /
PLOG/ 10.0 1.70E+38 -7.64 224.17 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH2NO+Hr=CH3r+NO
4.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH2NO+Hr=HCNO+H2
4.80E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+Or=CH2O+NO

7.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+Or=HCNO+HOr

3.30E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+HOr=CH2OH+NO

4.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+HOr=HCNO+H2O

2.40E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+O2=CH2O+NO2

1.10E+23 -3.29 16.30 ! T=900-2500 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+CH3r=C2H5r+NO

3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+CH3r=HCNO+CH4

1.60E+06 1.87 -4.66 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+H2Nr=CH4Nr+NO

3.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2NO+H2Nr=HCNO+H3N

1.80E+06 1.94 -4.82 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

!

C2H5r+NO=C2H5NO

1.40E+11 0.00 0.00 !

! G Pratt I Veltman J Chem Soc Faraday Trans 172 (1976) 2477-2483
!
C2H5NO+Hr=>C2H4_Olef+NO+H2
9.80E+13 0.00 38.58 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est C2H6+H; CH2CH2NO not stable
!
C2H5NO+Hr=CH3CHNO+H2
4.40E+08 1.50 1.58 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est CH3NO+H
!
C2H5NO+Or=>C2H4_Olef+NO+HOr
1.10E-07 6.50 1.15 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est C2H6+O CH2CH2NO not stable
!
C2H5NO+Or=CH3CHNO+HOr
3.30E+08 1.50 15.13 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est CH3NO+O
!
C2H5NO+HOr=>C2H4_Olef+NO+H2O
9.20E+06 2.00 4.14 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est C2H6+OH CH2CH2NO not stable
!
C2H5NO+HOr=CH3CHNO+H2O
3.60E+06 2.00 -4.99 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est CH3NO+OH
!
C2H5NO+HO2r=>C2H4_Olef+NO+H2O2
1.10E+05 2.50 70.50 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est C2H6+HO2 CH2CH2NO not stable
!
C2H5NO+O2=>C2H4_Olef+NO+HO2r
7.30E+05 2.50 205.69 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est C2H6+O2 CH2CH2NO not stable
!

!
 CH3CHNO=C2H4_Olef+NO
 2.00E+13 0.00 92.05 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3CH->C2H4
 !

CH2CHNO+Hr=CHCHNO+H2
 4.40E+08 1.50 1.58 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+H
 !

CH2CHNO+Hr=C2H3r_Olef+HNO
 1.80E+13 0.00 11.64 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+H
 !

CH2CHNO+Or=CHCHNO+HOr
 3.30E+08 1.50 15.13 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+O
 !

CH2CHNO+Or=C2H3r_Olef+NO2
 1.70E+08 2.08 0.00 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+O
 !

CH2CHNO+HOr=CHCHNO+H2O
 3.60E+06 2.00 -4.99 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+OH
 !

CH2CHNO+HOr=C2H3r_Olef+HONO
 2.50E+12 0.00 4.16 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
 (2011) 449-457
 ! est CH3NO+OH
 !

CHCHNO=C2H2+NO
 1.00E+14 0.00 3.72 !

! Nguyen HMT Sumathi R Nguyen MT J Phys Chem A 103 5015-5022 1999
 !
 !

CH3NO2 (+M)=CH3r+NO2 (+M)
 1.80E+16 0.00 244.76 !

LOW/ 1.26E+17 0.00 175.73 /
 TROE/ 0.183 1.0E-30 1.0E30 /

! Glänzer K Troe J Ber. Bunsen-Ges. Phys. Chem. 78:182 1974
 ! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
 !
 CH3NO2+Hr=CH3r+HNO2
 3.30E+12 0.00 15.61 !

! Ko T Fontijn A JPC 95:3984-3987 1991
 ! Thomsen EL Nielsen OJ Egsgaard H Chem Phys Lett 1993, 215, 257
 ! K Zhang Y Li T Yuan J Cai P Glarborg F Qi PCI 33 (2011) 407-414 (change products)
 !
 CH3NO2+Hr=CH3NO+HOr
 1.40E+12 0.00 15.61 !

! Ko T Fontijn A JPC 95:3984-3987 1991
 ! Thomsen EL Nielsen OJ Egsgaard H Chem Phys Lett 1993, 215, 257
 !
 CH3NO2+Hr=CH2NO2+H2
 4.90E+13 0.00 38.58 !

! K Zhang Y Li T Yuan J Cai P Glarborg F Qi PCI 33 (2011) 407-414
 !
 CH3NO2+Or=CH2NO2+HOr
 1.50E+13 0.00 22.38 !

! Sutter LF Thrush BA J Chem Soc Faraday Trans 1 1997, 73, 2025
 !
 ! CH3NO2+OH=CH3OH+NO2 2.0E10 0.000 -1000 !
 GLA/BEN99 GLA/BEN99 1 atm
 ! CH3NO2+OH=CH3OH+NO2 2.0E09 0.000 -1000 !
 GLA/BEN99 GLA/BEN99 0.1 atm
 !
 CH3NO2+HOr=CH2NO2+H2O
 5.00E+05 2.00 4.18 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
 ! JAM est
 !
 CH3NO2+HO2r=CH2NO2+H2O2
 3.00E+12 0.00 96.23 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
 ! est A factor, Ea = endothermicity+3kcal (as CH3OH+HO2)
 !
 CH3NO2+O2=CH2NO2+HO2r
 2.00E+13 0.00 238.49 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
 ! est A factor as CH3OH+O2, Ea = endothermicity
 !
 CH3NO2+CH3r=CH2NO2+CH4
 5.50E-01 4.00 34.73 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
 ! est C2H6+CH3

```

!
CH3NO2+CH3O=CH2NO2+CH3OH
      3.00E+11    0.00 29.29 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
CH3NO2+NO2=CH2NO2+HONO
      3.00E+11    0.00 133.89    !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
!
CH2NO2=CH2O+NO
      1.00E+13    0.00 150.62    ! 1 atm
PLOG/ 0.05    5.00E+11    0.00 150.62    /
PLOG/ 1.0     1.00E+13    0.00 150.62    /

! JC Tricot A Perche M Lucquin CF 40 (1981) 269-291
! K Zhang Y Li T Yuan J Cai P Glarborg F Qi PCI 33 (2011) 407-414
!
CH2NO2+Hr=CH3r+NO2
      5.00E+13    0.00 0.00    !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
CH2NO2+Or=CH2O+NO2
      5.00E+13    0.00 0.00    !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
CH2NO2+HOr=CH2OH+NO2
      1.00E+13    0.00 0.00    !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
CH2NO2+HOr=CH2O+HONO
      1.00E+13    0.00 0.00    !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999
!
!!CH2NO2+CH3r=C2H5r+NO2
      5.00E+13    0.00 0.00    !

! K Zhang Y Li T Yuan J Cai P Glarborg F Qi PCI 33 (2011) 407-414
!
!
C2H5NO2=C2H5r+NO2
      2.20E+66   -15.49    321.15    ! 1 atm
PLOG/ 0.01    3.00E+62   -15.03    298.37    /
PLOG/ 0.046   8.90E+64   -15.52    307.58    /
PLOG/ 0.1     5.60E+65   -15.64    311.72    /
PLOG/ 1.0     2.20E+66   -15.49    321.15    /
PLOG/ 10.0    8.60E+63   -14.48    324.44    /

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
!

```

C2H5NO2=C2H4_Olef+HNO2

6.90E+67	-16.52	298.99	!	1 atm	
PLOG/ 0.01	2.80E+80	-20.74	310.16	/	
PLOG/ 0.046	1.10E+77	-19.55	308.08	/	
PLOG/ 0.1	9.70E+74	-18.87	306.40	/	
PLOG/ 1.0	6.90E+67	-16.52	298.99	/	
PLOG/ 10.0	1.00E+59	-13.71	287.52	/	

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

!

C2H5NO2=CH2CHNO+H2O

8.90E+51	-20.02	386.51	!
----------	--------	--------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

!

C2H5NO2=CH3CNO+H2O

1.1E48	-18.364	85601	!
--------	---------	-------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

!

C2H5NO2=CH3CH2ONO

2.10E+10	1.00	253.80	!
----------	------	--------	---

! Q Wang D Ng MS Mannan, Ind. Eng. Chem. Res. 48 (2009) 8745-8751

!

C2H5NO2+Hr=CH2CH2NO2+H2

9.80E+13	0.00	38.58	!
----------	------	-------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

! est C2H6+H

!

C2H5NO2+Hr=CH3CHNO2+H2

2.60E+07	1.65	11.83	!
----------	------	-------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

! est C2H5OH+H

!

C2H5NO2+Hr=C2H5NO+HOr

1.40E+12	0.00	15.61	!
----------	------	-------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

! est CH3NO2+H

!

C2H5NO2+Or=CH2CH2NO2+HOr

1.10E-07	6.50	1.15	!
----------	------	------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

! est C2H6+O

!

C2H5NO2+Or=CH3CHNO2+HOr

1.90E+07	1.85	7.63	!
----------	------	------	---

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H5OH+O
!
C2H5NO2+HO_r=CH2CH2NO2+H2O
9.20E+06 2.00 4.14 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H6+OH
!
C2H5NO2+HO_r=CH3CHNO2+H2O
4.60E+11 0.15 0.00 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H5OH+OH
!
C2H5NO2+HO_r=CH3CH2OH+NO2
2.00E+10 0.00 -4.18 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est CH3NO2+OH=CH3OH+NO2
!
C2H5NO2+HO2_r=CH2CH2NO2+H2O2
1.10E+05 2.50 70.50 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H6+HO2
!
C2H5NO2+HO2_r=CH3CHNO2+H2O2
8.20E+03 2.55 44.98 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H5OH+HO2
!
C2H5NO2+O2=CH2CH2NO2+HO2_r
7.30E+05 2.50 205.69 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H6+O2
!
C2H5NO2+CH3_r=CH2CH2NO2+CH4
2.20E+02 3.18 40.26 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624
! est C2H5OH+CH3
!
C2H5NO2+CH3_r=CH3CHNO2+CH4
7.30E+02 2.99 33.25 !

! K Zhang L Zhang M Xie LI Ye F Zhang P Glarborg F Qi; Proc Combust Inst
34 (2013) 617-624

! est C2H5OH+CH3
!
C2H4_Olef+NO2=CH2CH2NO2
9.40E+11 0.00 58.58 !

! JL Sprung H Akimoto JN Pitts J Am Chem Soc 96 (1974) 6549-6554
!
CH3CHNO2=C2H4_Olef+NO2
2.00E+13 0.00 92.05 !

! J Giménez-López MU Alzueta CL Rasmussen P Marshall P Glarborg; PCI 33
(2011) 449-457
! est CH3CH->C2H4
!
!
CH3O+NO(+M)=CH3ONO(+M)
6.00E+14 -0.60 0.00 !
LOW/ 8.14E+25 -2.80 0.00 /
TROE/ 1.0 1.0E-30 900.0 1.0E30 /

! Caralp F Rayez M-T Forst W Gomez N Delcroix B Fittschen C Devolder P
JCSFT 94:3321-3330 1998
!
CH3ONO+Hr=CH3OH+NO
1.20E+11 0.00 7.95 !

! Moortgat GK Slemr F Warneck P IJCK 9:249 1977
!
CH3ONO+Hr=CH2O+H2+NO
1.40E+11 0.00 7.95 !

! Moortgat GK Slemr F Warneck P IJCK 9:249 1977
!
CH3ONO+Or=CH3O+NO2
1.40E+13 0.00 21.80 !

! Davidson JA Thrush BA JCS-FT I 71:2413 1975
!
CH3ONO+HOR=CH3OH+NO2
6.00E+13 0.00 14.66 !

! Nielsen OJ Sidebottom HW Donlon M Treacy J IJCK 23:1095-1109 1991
!
!
CH3CH2O+NO(+M)=CH3CH2ONO(+M)
1.20E+13 0.00 -0.60 !
LOW/ 9.43E+19 0.00 0.00 /
TROE/ 0.6 1.0E-30 1.0E30 1.0E30 /

! Daële V Ray A Vassalli I Poulet G Le Bras G IJCK 27:1121-1133 1995
! Fittschen C Frenzel A Imrik K Devolder P IJCK 31:860-866 1999
! Atkinson R Baulch DL Cox RA Crowley JN Hampson RF Hynes RG Jenkin ME
Rossi MJ Troe JACP 6:3625-4055 2006
!
CH3CH2ONO+HOR=CH3CH2OH+NO2
1.60E+14 0.00 14.66 !

! Nielsen OJ Sidebottom HW Donlon M Treacy J Int. J. Chem. Kinet. 23
1095-1109 1991

!
!

CH3O+NO2 (+M)=CH3ONO2 (+M)

2.20E+15 -0.88 0.00 !
LOW/ 2.91E+23 -1.74 0.00 /
TROE/ 0.6 1.0E-30 1.0E30 1.0E30 /

! Martínez E Albaladejo J Jiménez E Notario A de Mera D 2000

!

CH3ONO2+Hr=CH3O+HONO

1.00E+12 0.00 0.00 !

! Glarborg P Bendtsen AB Miller JA IJCK 31:591-602 1999

!

CH3ONO2+Or=CH3O+NO3

1.50E+13 0.00 22.01 !

! Salter LF Thrush BA JCSFT 1, 1098, 1977

!

CH3ONO2+HOr=CH3O+HONO2

4.90E+11 0.00 8.48 !

! Talukdar RK Herndon SC Burkholder JB Roberts JM Ravishankara AR JCSFT
93:2787-2796 1997

!

!

CH3CH2O+NO2 (+M)=CH3CH2ONO2 (+M)

5.10E+15 -1.00 0.00 !
LOW/ 5.88E+30 -4.00 0.00 /
TROE/ 0.6 1.0E-30 1.0E30 1.0E30 /

! DeMore WB Sander SP Golden DM Hampson RF Kurylo MJ Howard CJ
Ravishankara AR Kolb CE Molina MJ JPL Pub. 97-4 1997

!

CH3CH2ONO2+HOr=CH3CH2O+HONO2

2.20E+12 0.00 8.95 ! RAS/GLA08d TAL/RAV97

DUP

CH3CH2ONO2+HOr=CH3CH2O+HONO2

3.20E+10 0.00 -1.05 !

DUP

! Talukdar RK Herndon SC Burkholder JB Roberts JM Ravishankara AR J Chem
Soc Faraday Trans 93 2787-2796 1997

!

!

!

! Amino hydrocarbon subset

*

!

!

CH3r+H2Nr=CH5N

5.10E+52 -11.99 70.25 ! 1 atm

PLOG/ 0.1 1.30E+54 -12.72 65.30 /
PLOG/ 1.0 5.10E+52 -11.99 70.25 /
PLOG/ 10.0 1.60E+47 -10.15 65.63 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
!CH3NH2+M=CHNH2+H2+M 1.3E14 0.000 82560 !
! Zhang RQ Han KL Zhu RS Lee CS Lee ST CPL 321:101-105 2000
!
CH5N+M=CH3N+H2+M
2.40E+13 0.00 448.78 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3r+H2Nr=CH4Nr+Hr
1.40E+14 -0.43 46.47 ! 1 atm
PLOG/ 0.1 1.10E+13 -0.13 41.44 /
PLOG/ 1.0 1.40E+14 -0.43 46.47 /
PLOG/ 10.0 7.40E+12 0.00 50.51 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3r+H2Nr=CH4Nr_1+Hr
4.40E+13 -0.31 69.63 ! 1 atm
PLOG/ 0.1 1.20E+13 -0.15 67.55 /
PLOG/ 1.0 4.40E+13 -0.31 69.63 /
PLOG/ 10.0 1.40E+14 -0.42 74.74 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH3r+H2Nr=CH3N+H2
4.80E+11 -0.20 81.18 ! 1 atm
PLOG/ 0.1 2.10E+11 -0.10 79.89 /
PLOG/ 1.0 4.80E+11 -0.20 81.18 /
PLOG/ 10.0 2.90E+12 -0.40 85.80 /

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH4Nr+Hr=CH3N+H2
4.80E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH4Nr+Or=CH2O+H2Nr
7.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!
CH4Nr+Or=CH3N+HO
3.30E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr+HOr=CH2OH+H2Nr
4.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr+HOr=CH3N+H2O
2.40E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

!CH2NH2+O2=NH2CH2O+O 6.0E18 -1.590 30192 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr+O2=CH3N+HO2r
1.00E+22 -3.09 28.27 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr+CH3r=C2H5r+H2Nr
2.00E+13 0.00 11.31 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr+CH3r=CH3N+CH4
1.60E+06 1.87 -2.62 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr_1+Hr=CH3N+H2
7.20E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr_1+Or=CH3N+HOr
5.00E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr_1+HOr=CH3N+H2O
3.60E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH4Nr_1+CH3r=CH3N+CH4
2.40E+06 1.87 -4.66 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH3N+Or=CH2Nr+HOr
1.70E+08 1.50 19.37 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH3N+Or=CHNHr+HOr
2.20E+08 1.50 22.61 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH3N+Or=CH2O+NH
1.70E+06 2.08 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH3N+CH3r=CH2Nr+CH4
8.20E+05 1.87 29.80 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2Nr+Hr=HCN+H2
2.40E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2Nr+Or=HCN+HOr
1.70E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2Nr+HOr=HCN+H2O
1.50E+19 -2.18 9.06 ! 1 atm
PLOG/ 0.1 2.10E+17 -1.68 1.33 /
PLOG/ 1.0 1.50E+19 -2.18 9.06 /
PLOG/ 10.0 9.50E+21 -2.91 23.57 /

DUP

CH2Nr+HOr=HCN+H2O
1.20E+06 2.00 -4.99 ! 1 atm
PLOG/ 0.1 1.20E+06 2.00 -4.99 /
PLOG/ 1.0 1.20E+06 2.00 -4.99 /
PLOG/ 10.0 1.20E+06 2.00 -4.99 /

DUP

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH2Nr+O2=CH2O+NO
3.00E+12 0.00 24.94 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH₂N_r+H₂N_r=HCN+H₃N
9.20E+05 1.94 -4.82 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CH₂N_r+NH=HCN+H₂N_r
1.70E+08 1.50 -3.74 !

! est H₂CN+O

!

CH₂N_r+N=CH₂+N₂
2.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+H_r=CH₂N_r+H_r
2.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+H_r=HCN+H₂
2.40E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+O_r=HNCO+H_r
7.00E+13 0.00 0.00 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+O_r=HCN+H_O
1.70E+08 1.50 -3.74 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+H_O=HCN+H₂O
1.20E+06 2.00 -4.99 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

CHNH_r+CH₃_r=HCN+CH₄
8.20E+05 1.87 -4.66 !

! Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry,
Springer 2000

!

!

C2H7N=C2H4_Olef+H3N
 6.20E+67 -15.94 415.67 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! 0.04 bar, 1000-2500 K
 !

C2H5r+H2Nr(+M)=C2H7N(+M)
 7.20E+12 0.42 0.00 !
 LOW/ 2.20E+30 -3.85 0.00 /

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3+nh2
 !

C2H6Nr_2+Hr=C2H7N
 1.70E+13 0.22 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est i-c3h7+h
 !

C2H6Nr_3+Hr=C2H7N
 5.40E+13 0.16 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est c2h5+h
 !

C2H7N+Hr=C2H6Nr_3+H2
 1.20E+07 1.80 21.34 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+h
 !

C2H7N+Hr=C2H6Nr_2+H2
 2.60E+07 1.65 11.84 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+h
 !

C2H7N+Hr=C2H6Nr+H2
 4.80E+08 1.50 40.58 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+h
 !

C2H7N+Or=C2H6Nr_3+HOr
 9.40E+07 1.70 22.84 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+o
 !

$C_2H_7N+Or=C_2H_6Nr_2+HOr$
 6.80E+12 0.00 5.33 !

! R Atkinson JN Pitts Jr J Chem Phys 68 (1978) 911-915 (ktot)
 !

$C_2H_7N+Or=C_2H_6Nr+HOr$
 3.30E+08 1.50 26.56 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+o
 !

$C_2H_7N+HOr=C_2H_6Nr_3+H_2O$
 7.94E+02 2.97 -0.44 !

! Adapted value from Li et al.
 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+oh
 ! 1.6E12 0.000 1300
 !

$C_2H_7N+HOr=C_2H_6Nr_2+H_2O$
 3.28E+02 2.24 -12.73 !

! Adapted value from Li et al.
 ! SA Carl JN Crowley JPCA 102 (1998) 8131-8141 (products)
 ! 1.4E13 0.000 0
 !

$C_2H_7N+HOr=C_2H_6Nr+H_2O$
 1.12E+05 2.36 -11.96 !

! Adapted value from Li et al.
 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+oh - minor ch in agr with GALALV08 theory
 ! 2.4E06 2.000 447
 !

$C_2H_7N+HO_2r=C_2H_6Nr_3+H_2O_2$
 1.20E+04 2.55 65.90 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+ho2
 !

$C_2H_7N+HO_2r=C_2H_6Nr_2+H_2O_2$
 8.20E+03 2.55 44.98 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+ho2
 !

$C_2H_7N+CH_3r=C_2H_6Nr_3+CH_4$
 2.20E+02 3.18 40.25 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est C2H5OH+ch3
 !

C2H7N+CH3r=C2H6Nr_2+CH4
7.30E+02 2.99 33.26 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est C2H5OH+ch3

!

C2H7N+CH3r=C2H6Nr+CH4
1.60E+06 1.87 36.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+ch3

!

C2H7N+H2Nr=C2H6Nr_3+H3N
2.20E+02 3.18 40.25 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est C2H5OH+ch3

!

C2H7N+H2Nr=C2H6Nr_2+H3N
7.30E+02 2.99 33.26 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est C2H5OH+ch3

!

C2H7N+H2Nr=C2H6Nr+H3N
1.80E+06 1.94 29.87 !

! P.V. Khe, R. Lesclaux, J. Phys. Chem. 83 (1979) 1119-1122 (addition,
close to hpl)

!

C2H6Nr_3+Hr=C2H5N_Olef+H2
1.80E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+Or=CH2O+CH4Nr
9.60E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+HOR=C2H5N_Olef+H2O
2.40E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+HO2r=>CH2O+HOR+CH4Nr
2.40E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+O2=C2H5N_Olef+HO2r
3.70E+16 -1.63 14.30 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+HCO=C2H7N+CO
6.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est n-c3h7

!

C2H6Nr_3+CH3r=C2H5N_Olef+CH4
1.20E+13 -0.32 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est c2h4+h(+m)

!

C2H6Nr_2=CH3CHNH+Hr
1.10E+45 -10.24 200.07 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2

!

C2H6Nr_2+Hr=C2H5N_Olef+H2
4.90E+08 1.70 2.46 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3choh

!

C2H6Nr_2+Hr=CH3r+CH4Nr
8.40E+16 -0.89 12.15 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3choh

!

C2H6Nr_2+Hr=C2H4_Olef+H3N
4.70E+21 -3.02 11.90 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3choh

!

C2H6Nr_2+Hr=C2H5r+H2Nr
2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est i-c3h7
!
C2H6Nr_2+Or=CH3r+H2NCHO
4.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+Or=C2H5N_Olef+HOr
2.50E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+HOr=C2H5N_Olef+H2O
2.40E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+HO2r=>CH3r+HOr+H2NCHO
2.40E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+O2=C2H5N_Olef+HO2r
6.70E+20 -3.02 10.48 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+HCO=C2H7N+CO
1.20E+14 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est i-c3h7
!
C2H6Nr_2+CH3r=C2H5N_Olef+CH4
1.80E+13 0.00 -3.22 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3ch2o, 0.04 bar, Ea+8
!
C2H6Nr=CH3CHNH+Hr
1.60E+36 -7.92 152.05 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh
!

C2H6Nr+Hr=CH3r+CH4Nr
1.40E+12 0.70 1.45 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3ch2o+h
!

C2H6Nr+Hr=CH3CHNH+H2
7.20E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh+h
!

C2H6Nr+Or=CH3CHNH+HOr
5.00E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh+o
!

C2H6Nr+HOr=CH3CHNH+H2O
3.60E+06 2.00 -4.99 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh+oh
!

C2H6Nr+CH3r=CH3CHNH+CH4
2.40E+06 1.87 -4.66 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh+ch3
!

CHCHNH2+Hr(+M)=C2H5N_Olef(+M)
3.90E+13 0.20 0.00 !
LOW/ 2.10E+24 -1.30 0.00 /
TROE/ 0.5 1.0E-30 1.0E30 1.0E30 /

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+h(+m)
!

C2H4Nr_Olef_2+Hr(+M)=C2H5N_Olef(+M)
3.90E+13 0.20 0.00 !
LOW/ 2.10E+24 -1.30 0.00 /
TROE/ 0.5 1.0E-30 1.0E30 1.0E30 /

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+h(+m)
!

C2H5N_Olef+Hr=CHCHNH2+H2
2.40E+02 3.63 47.14 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.


```

! est ch3nh2+h
!
C2H5N_Olef+Or=CH3r+H2NCO
      3.90E+12    0.00 6.25 !
DUP
C2H5N_Olef+Or=CH3r+H2NCO
      6.20E+13    0.00 28.68 !
DUP

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+o
!
C2H5N_Olef+HOr=CHCHNH2+H2O
      1.30E-01    4.20 -3.60 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+oh
!
C2H5N_Olef+CH3r=CHCHNH2+CH4
      6.00E+07    1.56 69.58 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+ch3
!
C2H5N_Olef+H2Nr=CHCHNH2+H3N
      5.30E+12    0.00 42.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h4+nh2
!
C2H5N_Olef+H2Nr=C2H4Nr_Olef_2+H3N
5.30E+12    0.00 42.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+nh2
!
CH3CHNH=C2H5N_Olef
      5.00E+18   -2.50 284.49    !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! 0.04 bar, 1300-3000 K
!
C2H4Nr_2+Hr=CH3CHNH
      5.80E+13    0.18 -0.52 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2chch2+h
!
CH3r+CHNHr=CH3CHNH
      1.80E+13    0.00 0.00 !

```

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3+hco

!

CH3CHNH+Hr=C2H5N_{olef}+Hr

3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

CH3CHNH+Hr=C2H4Nr₃+H2

4.70E+13 -0.35 12.55 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+h

!

CH3CHNH+Hr=C2H4Nr₂+H2

1.90E+12 0.40 22.42 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+h

!

CH3CHNH+Hr=C2H4Nr₄+H2

2.40E+08 1.50 30.64 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+h

!

CH3CHNH+Or=C2H4Nr₃+HOr

1.80E+18 -1.90 12.45 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+o

!

CH3CHNH+Or=C2H4Nr₂+HOr

3.70E+13 -0.20 14.88 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+o

!

CH3CHNH+Or=C2H4Nr₄+HOr

1.70E+08 1.50 19.37 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+o

!

CH3CHNH+HOr=C2H4Nr₃+H2O

2.40E+11 0.30 -4.18 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+oh

!

CH3CHNH+HOr=C2H4Nr_2+H2O

3.00E+13 -0.60 3.35 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+oh

!

CH3CHNH+HOr=C2H4Nr_4+H2O

1.20E+06 2.00 -0.37 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+oh

!

CH3CHNH+CH3r=C2H4Nr_3+CH4

3.90E-07 5.80 9.20 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+ch3

!

CH3CHNH+CH3r=C2H4Nr_2+CH4

2.50E+01 3.15 23.96 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3hco+ch3

!

CH3CHNH+CH3r=C2H4Nr_4+CH4

8.20E+05 1.87 29.80 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+ch3

!

CH3CHNH+H2Nr=C2H4Nr_4+H3N

9.20E+05 1.94 18.58 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+nh2

!

H2Nr+C2H2=CHCHNH2

7.80E-18 8.31 31.09 !

! L.V. Moskaleva, M.C. Lin, J. Phys. Chem. A 102 (1998) 4687-4693
ktot(350mbar)

!

CHCNH2+Hr(+M)=CHCHNH2(+M)

1.70E+10 1.27 11.33 !

LOW/ 6.30E+31 -4.66 15.82 /

TROE/ 0.7878 -10212.0 1.0E30 /

CO/ 2.0/ CO2/ 3.0/ H2/ 2.0/ H2O/ 5.0/

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K Kohse-Höinghaus, CF 159 (2012) 2254-2279.

```

! est c2h2+h(+m)
!
CHCHNH2+Hr=CHCNH2+H2
      4.50E+13    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+h
!
! CHCHNH2+O=OCCHNH2+H                3.0E13    0.000    0  !
! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+o
!
CHCHNH2+HOr=CHCNH2+H2O
      2.00E+13    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+oh
!
CHCHNH2+O2=OCHCHO+H2Nr
      4.00E+12    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est chchoh+o2
!
CHCHNH2+CH3r=CHCNH2+CH4
      2.00E+13    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+ch3
!
CHCNH2+Hr(+M)=C2H4Nr_Olef_2(+M)
      1.70E+10    1.27 11.33  !
      LOW/   6.30E+31   -4.66 15.82 /
      TROE/  0.7878    -10212.0   1.0E30   /
      CO/    2.0/   CO2/  3.0/   H2/    2.0/   H2O/  5.0/

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h2+h(+m)
!
C2H4Nr_Olef_2+Hr=CHCNH2+H2
      4.50E+13    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+h
!
C2H4Nr_Olef_2+Or=CH2CO+H2Nr
      3.00E+13    0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est c2h3+o

```

!
 C2H4Nr_Olef_2+HOr=CHCNH2+H2O
 2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est c2h3+oh
 !

C2H4Nr_Olef_2+O2=OCHCHO+H2Nr
 4.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est chcho+o2
 !

C2H4Nr_Olef_2+CH3r=CHCNH2+CH4
 2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est c2h3+ch3
 !

C2H4Nr_2+Hr=CH3r+CHNHr
 1.00E+14 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2cho+h
 !

C2H4Nr_2+Hr=C2H4Nr_3+Hr
 3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2cho+h
 !

C2H4Nr_2+Hr=CH2CNH+H2
 2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2cho+h
 !

C2H4Nr_2+Or=CH2CNH+HOr
 2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2cho+o
 !

C2H4Nr_2+HOr=CH2CNH+H2O
 2.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2cho+oh
 !

C2H4Nr_2+HOr=CH2OH+CHNHr
1.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2cho+oh

!

C2H4Nr_2+O2=CH2O+CO+H2Nr
5.70E+17 -1.76 46.30 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2cho+o2 (1 atm)

!

C2H4Nr_3=CH3r+HNC
6.50E+18 -2.52 138.07 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est hcnh; Ea+2 0.1 atm

!

C2H4Nr_3+Hr=CH3r+CHNHr
2.10E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+h

!

C2H4Nr_3+Hr=CH2CNH+H2
1.20E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+h

!

C2H4Nr_3+Hr=CH3CN+H2
2.40E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est hcnh+h

!

C2H4Nr_3+Or=CH3r+HNCO
1.60E+14 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+o

!

C2H4Nr_3+Or=CH2CNH+HOr
5.30E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+o

!

C2H4Nr_3+Or=CH3CN+HOr
1.70E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est hcnh+o

!

C2H4Nr_3+HOr=CH2CNH+H2O
1.20E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+oh

!

C2H4Nr_3+HOr=CH3CN+H2O
1.20E+06 2.00 -4.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est hcnh+oh

!

C2H4Nr_3+O2=CH2O+CO+H2Nr
1.90E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+o2

!

C2H4Nr_3+CH3r=CH2CNH+CH4
5.30E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3co+ch3

!

C2H4Nr_3+CH3r=CH3CN+CH4
8.20E+05 1.87 -4.66 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est hcnh+ch3

!

!!CH3r+HCN=C2H4Nr_4
1.00E+12 0.00 41.42 !

C2H4Nr_4=CH3r+HCN
1.4E+14 0.00 124.6 !

! B Wang H Hou Y Gu J Phys Chem A 105 (2001) 156-164

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

C2H4Nr_4+Hr=CH3CN+H2
2.40E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est h2cn+h

!

C2H4Nr_4+Hr=CH2CHN(S)+H2
9.00E+13 0.00 63.18 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3+h

!

CH2CHN(S)_m0+H2=C2H4Nr_4+Hr
7.20E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2(s)+h2

!

C2H4Nr_4+Or=CH3CN+HOr
1.70E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est h2cn+o

!

C2H4Nr_4+HOr=CH3CN+H2O
1.20E+06 2.00 -4.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est h2cn+oh

!

C2H4Nr_4+HOr=CH2CHN(S)+H2O
1.10E+03 3.00 11.63 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3+oh

!

C2H4Nr_4+HOr=CH2CHN(S)_m0+H2O
4.40E+13 -0.35 -3.04 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3+oh

!

C2H4Nr_4+H2Nr=CH3CN+H3N
9.20E+05 1.94 -4.82 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est h2cn+nh2

!

CHCNH2+Hr=CHCNH+H2
4.80E+08 1.50 40.61 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+h

!

CHCNH2+Or=CHCNH+HOr
3.30E+08 1.50 26.56 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+o

!

CHCNH2+Or=HCCO+H2Nr

1.40E+07 2.00 7.95 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est c2h2+o

!

CHCNH2+HOr=CHCNH+H2O

2.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+oh

!

CHCNH2+CH3r=CHCNH+CH4

1.60E+06 1.87 36.99 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+ch3

!

CHCNH2+H2Nr=CHCNH+H3N

1.80E+06 1.94 29.89 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+nh2

!

CH2CNH=CH3CN

2.50E+13 0.00 294.14 !

! A. Doughty, G.B. Bacskay, J.C. Mackie, J. Phys. Chem. 98 (1994) 13546-
13555

!

CH2CNH+Hr=CH3CN+Hr

3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

CH2CNH+Hr=CH3r+HNC

3.30E+10 0.85 11.88 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2co+h

!

CH2CNH+Hr=CHCNH+H2

3.00E+07 2.00 41.84 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2co+h
!
CH2CNH+Hr=C2H2Nr+H2
2.40E+08 1.50 30.64 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2nh+h
!
CH2CNH+Or=CH2+HNCO
1.80E+12 0.00 5.65 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2co+o
!
CH2CNH+Or=CHCNH+HOr
2.00E+07 2.00 41.84 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2co+o
!
CH2CNH+Or=C2H2Nr+HOr
1.70E+08 1.50 19.37 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2nh+o
!
CH2CNH+HOr=CH2OH+HNC
1.00E+12 0.00 -4.24 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2co+oh
!
CH2CNH+HOr=CH3r+HNCO
6.70E+11 0.00 -4.24 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2co+oh
!
CH2CNH+HOr=CHCNH+H2O
1.00E+07 2.00 12.55 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2co+oh
!
CH2CNH+HOr=C2H2Nr+H2O
1.20E+06 2.00 -0.37 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2nh+oh
!

CH2CNH+CH3r=C2H2Nr+CH4
8.20E+05 1.87 29.80 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2nh+ch3
!

CH2CNH+H2Nr=C2H2Nr+H3N
9.20E+05 1.94 18.58 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2nh+nh2
!

CH2CHN(S)+Hr=CH3r+HCN
1.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

CH2CHN(S)+Or=CH2O+HCN
5.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

CH2CHN(S)+O2=CH2O+HNCO
1.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

CH2CHN(S)_m0+M=CH2CHN(S)+M
1.00E+13 0.00 0.00 !
Hr/ 0.0/

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2(s)
!

CH2CHN(S)_m0+Hr=CH2CHN(S)+Hr
1.00E+14 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch2(s)
!

CH2CHN(S)_m0+Hr=CH3r+HCN
3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

CH2CHN(S)_m0=c-C2H3N
3.00E+13 0.00 16.74 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est
!

CH2CHN(S)_m0=CH3CN
3.00E+13 0.00 33.47 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est
!

CH2CHN(S)_m0+Or=>HCO+HCN+Hr
3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est
!

CH2CHN(S)_m0+HOr=>CH2O+HCN+Hr
3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!

c-C2H3N+Hr=C2H4Nr_1
9.80E+09 1.21 8.24 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!

c-C2H3N+Hr=C2H4Nr_2
1.10E+10 1.23 10.13 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!

c-C2H3N+Or=>CH2Nr+HCO
1.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est
!

c-C2H3N+Or=>C2H3r_Olef+NO
1.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est
!

c-C2H3N+HOr=>CH2Nr+CH2O
5.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

```

! est
!
CHCNH+Hr=CH2+HNC
      1.50E+14   0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+h
!
CHCNH+Or=Hr+CO+HNC
      1.00E+14   0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+o
!
CHCNH+HOr=HCO+CHNHr
      1.00E+13   0.00 0.00  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+oh
!
CHCNH+O2=HNCO+HCO
      4.90E+12  -0.14 4.81  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+o2
!
CHCNH+O2=HNC+CO+HOr
      1.60E+11  -0.02 4.27  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+o2
!
CHCNH+O2=HNC+HCO+Or
      2.20E+02   2.69 14.81  !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est hcco+o2
!
H2NCHO (+M)=CO+H3N (+M)
      1.00E+14   0.00 315.95  !
LOW/  8.30E+14   0.00 205.37  /

! T Kakumoto K Saito A Imamura JPC 89 (1985) 2286-2291
!
H2NCHO+M=HCO+H2Nr+M
      1.40E+16   0.00 305.01  !

! T Kakumoto K Saito A Imamura JPC 89 (1985) 2286-2291
!
H2NCHO+M=H2NCO+Hr+M
      4.60E+15   0.00 268.61  !

```

! T Kakumoto K Saito A Imamura JPC 89 (1985) 2286-2291
!

H2NCHO+Hr=H2NCO+H2
1.30E+13 0.00 29.10 !

! EA Syrstad F Turecek JPCA 105 (2001) 11144-11155
!

H2NCHO+Hr=HCO+H3N
1.00E+13 0.00 79.91 !

! EA Syrstad F Turecek JPCA 105 (2001) 11144-11155
! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
!

H2NCHO+Or=H2NCO+HOr
4.00E+08 1.50 21.74 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+o
!

H2NCHO+HOr=H2NCO+H2O
8.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est ch3nh2+oh
!

H2NCHO+CH3r=H2NCO+CH4
7.00E+05 2.00 37.66 !

! J.C. Boden, R.A. Back, Trans. Faraday Soc. 66 (1970) 175-182
! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
!

H2NCHO+H2Nr=H2NCO+H3N
2.00E+06 2.00 20.92 !

! R.A. Back, T. Yokota, Int. J. Chem. Kinet. 5 (1973) 37-46 (573 K)
! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

H2NCO (+M)=CO+H2Nr (+M)
5.90E+12 0.00 104.60 !
LOW/ 1.00E+14 0.00 90.79 /

! R.A. Back, T. Yokota, Int. J. Chem. Kinet. 5 (1973) 37-46 (573 K)
!

H2NCO+Hr=HNCO+H2
3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.
! est
!

H2NCO+Or=HNCO+HOr
3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

H2NCO+HOr=HNCO+H2O

3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

!

C2H6Nr_1+Hr(+M)=CH3NHCH3(+M)

5.20E+17 -0.99 6.61 !

LOW/ 1.99E+41 -7.08 27.97 /

TROE/ 0.8422 125.0 2219.0 6882.0 /

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est c2h5+h(+m)

!

CH3NCH3+Hr=CH3NHCH3

1.00E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

CH3NHCH3+Hr=C2H6Nr_1+H2

5.60E+08 1.50 22.86 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+h

!

CH3NHCH3+Hr=CH3NCH3+H2

4.80E+08 1.50 40.61 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+h

!

CH3NHCH3+Or=C2H6Nr_1+HOr

6.10E+12 0.00 2.33 !

! R. Atkinson, R.A. Perry, J.N. Pitts Jr., J. Chem. Phys. 68 (1978) 1850-
1853 (overall rate)

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!

CH3NHCH3+Or=CH3NCH3+HOr

3.00E+12 0.00 2.33 !

! R. Atkinson, R.A. Perry, J.N. Pitts Jr., J. Chem. Phys. 68 (1978) 1850-
1853 (overall rate)

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!
 CH3NHCH3+HOr=C2H6Nr_1+H2O
 2.00E+13 0.00 0.00 !

 ! S.A. Carl, J.N. Crowley, J. Phys. Chem. A 102 (1998) 8131-8141
 ! A. Galano, R. Alvarez-Idaboy, J. Chem. Theory Comput. 4 (2008) 322-327
 !
 CH3NHCH3+HOr=CH3NCH3+H2O
 1.90E+13 0.00 0.00 !

 ! S.A. Carl, J.N. Crowley, J. Phys. Chem. A 102 (1998) 8131-8141
 ! A. Galano, R. Alvarez-Idaboy, J. Chem. Theory Comput. 4 (2008) 322-327
 !
 CH3NHCH3+CH3r=C2H6Nr_1+CH4
 1.50E+06 1.87 38.37 ! ch3nh2+ch3

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+ch3
 !
 CH3NHCH3+CH3r=CH3NCH3+CH4
 1.60E+06 1.87 36.99 ! ch3nh2+ch3

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+ch3
 !
 CH3NHCH3+H2Nr=C2H6Nr_1+H3N
 2.80E+06 1.94 22.99 !

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch3nh2+nh2
 !
 CH3NHCH3+H2Nr=CH3NCH3+H3N
 1.80E+06 1.94 29.89 !

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! 0.04 bar
 !
 C2H6Nr_1+Hr=C2H5N_2+H2
 4.80E+08 1.50 -3.74 !

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2nh2+h
 !
 C2H6Nr_1+Or=CH2O+CH4Nr_1
 7.00E+13 0.00 0.00 !

 ! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
 Kohse-Höinghaus, CF 159 (2012) 2254-2279.
 ! est ch2nh2+o
 !
 C2H6Nr_1+Or=C2H5N_2+HOr
 3.30E+08 1.50 -3.74 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2+o

!

C2H6Nr_1+HOr=CH2OH+CH4Nr_1
4.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2+oh

!

C2H6Nr_1+HOr=C2H5N_2+H2O
2.40E+06 2.00 -4.99 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2+oh

!

C2H6Nr_1+CH3r=C2H5r+CH4Nr_1
2.00E+13 0.00 11.31 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2+ch3

!

C2H6Nr_1+CH3r=C2H5N_2+CH4
1.60E+06 1.87 -2.62 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh2+ch3

!

CH3NCH3=C2H5N_2+Hr
1.60E+35 -7.54 160.77 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! 0.04 bar

!

CH3NCH3+Hr=C2H5N_2+H2
3.20E+12 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est i-c3h7

!

CH3NCH3+Or=CH3NO+CH3r
5.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

CH3NCH3+HOr=C2H5N_2+H2O
2.40E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est i-c3h7

!

CH3NCH3+O2=CH3NO+CH3O

1.00E+09 1.00 25.10 !

! C.R.C. Lindley, J.G. Calvert, J.H. Shaw, Chem. Phys. Lett. 67 (1979)
57-62

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

!

CH3NCH3+CH3r=C2H5N_2+CH4

6.00E+12 0.00 0.00 !

! J Seetula K Kalliorinne J Koskikallio J Photochem Photobiol A 43 (1988)
31-41

!

C2H4Nr_1+Hr=C2H5N_2

5.80E+13 0.18 -0.52 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+o f

!

C2H5N_2+Or=C2H4Nr+HOr

2.20E+08 1.50 22.61 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch2nh+ch3

!

C2H5N_2+H2Nr=C2H4Nr_1+H3N

2.80E+06 1.94 22.99 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est ch3nh2+nh2

!

C2H5N_2+H2Nr=C2H4Nr+H3N

1.80E+06 1.94 25.48 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! 0.04 bar, 700-3000 K

!

C2H4Nr_1+Hr=CH3r+CH2Nr

3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

C2H4Nr_1+Or=CH2O+CH2Nr

3.00E+13 0.00 0.00 !

! A Lucassen K Zhang J Warkentin K Moshhammer P Glarborg P Marshall K
Kohse-Höinghaus, CF 159 (2012) 2254-2279.

! est

!

C2H3r_Olef+C2H5N_Olef=C2H4_Olef+C2H4Nr_Olef_1
1.03E+13 0.00 64.30
C2H3r_Olef+C2H5N_Olef=C2H4_Olef+C2H4Nr_Olef_2
1.02E+13 0.00 58.40
C2H3r_Olef+C3H5N_Olef=C2H4_Olef+C3H4Nr_Olef
1.08E+13 0.00 64.30
C2H3r_Olef+C3H5N_Olef=C2H4_Olef+C3H4Nr_Olef_1
1.08E+13 0.00 64.30
C2H3r_Olef+C3H5N_Olef=C2H4_Olef+C3H4Nr_Olef_2
1.23E+13 0.00 41.30
C2H3r_Olef+C3H5N_Olef=C2H4_Olef+C3H4Nr_Olef_3
1.02E+13 0.00 58.40
C2H3r_Olef+C3H6_Olef=C2H4_Olef+C3H5r_Olef
5.80E+12 0.00 38.90
C2H3r_Olef+C3H6_Olef=C2H4_Olef+C3H5r_Olef_1
1.16E+13 0.00 55.10
C2H3r_Olef+C3H6_Olef=C2H4_Olef+C3H5r_Olef_2
1.07E+13 0.00 64.30
C2H3r_Olef+C3H6_Olef=C2H4_Olef+C3H5r_Olef_3
1.07E+13 0.00 64.30
C2H3r_Olef+C3H7N=C2H4_Olef+C3H6Nr_1
6.37E+12 0.00 37.80
C2H3r_Olef+C3H7N=C2H4_Olef+C3H6Nr_2
1.08E+13 0.00 36.30
C2H3r_Olef+C3H7N=C2H4_Olef+CH3CHNCH2
2.57E+13 0.00 40.50
C2H3r_Olef+C3H7N_1=C2H4_Olef+C3H6Nr_1
6.37E+12 0.00 37.80
C2H3r_Olef+C3H7N_1=C2H4_Olef+C3H6Nr_2
1.08E+13 0.00 36.30
C2H3r_Olef+C3H7N_1=C2H4_Olef+CH3CHNCH2
2.57E+13 0.00 40.50
C2H3r_Olef+C3H7N_2=C2H4_Olef+C3H6Nr_3
2.72E+13 0.00 53.90
C2H3r_Olef+C3H7N_2=C2H4_Olef+C3H6Nr_4
1.23E+13 0.00 41.30
C2H3r_Olef+C3H7N_2=C2H4_Olef+CH3CHNCH2
6.40E+12 0.00 36.60
C2H3r_Olef+C3H7N_Olef=C2H4_Olef+C3H6Nr_Olef
1.08E+13 0.00 64.30
C2H3r_Olef+C3H7N_Olef=C2H4_Olef+C3H6Nr_Olef_1
1.08E+13 0.00 64.30
C2H3r_Olef+C3H7N_Olef=C2H4_Olef+C3H6Nr_Olef_2
2.53E+13 0.00 43.40
C2H3r_Olef+C3H7N_Olef=C2H4_Olef+C3H6Nr_Olef_3
1.02E+13 0.00 58.40
C2H3r_Olef+C4H5N_Olef=C2H4_Olef+C4H4Nr_Olef
1.06E+13 0.00 64.30
C2H3r_Olef+C4H5N_Olef=C2H4_Olef+C4H4Nr_Olef_1
1.06E+13 0.00 64.30
C2H3r_Olef+C4H5N_Olef=C2H4_Olef+C4H4Nr_Olef_2
6.37E+12 0.00 37.80
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef
1.08E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_1
1.08E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_2
1.08E+13 0.00 64.30

C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_3
1.08E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_4
6.37E+12 0.00 37.80
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_5
1.02E+13 0.00 58.40
C2H3r_Olef+C4H7N_Olef=C2H4_Olef+C4H6Nr_Olef_6
1.08E+13 0.00 36.30
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef
1.06E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_1
1.06E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_2
1.06E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_3
1.06E+13 0.00 64.30
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_4
6.37E+12 0.00 37.80
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_5
1.02E+13 0.00 58.40
C2H3r_Olef+C4H7N_Olef_1=C2H4_Olef+C4H6Nr_Olef_6
1.08E+13 0.00 36.30
C2H3r_Olef+C4H8_Olef=C2H4_Olef+C4H7r_Olef
2.72E+13 0.00 53.90
C2H3r_Olef+C4H8_Olef=C2H4_Olef+C4H7r_Olef_1
1.07E+13 0.00 64.30
C2H3r_Olef+C4H8_Olef=C2H4_Olef+C4H7r_Olef_2
1.07E+13 0.00 64.30
C2H3r_Olef+C4H8_Olef=C2H4_Olef+C4H7r_Olef_3
1.16E+13 0.00 55.10
C2H3r_Olef+C4H8_Olef=C2H4_Olef+C4H7r_Olef_4
1.34E+13 0.00 30.80
C2H3r_Olef+C4H8_Olef_1=C2H4_Olef+C4H7r_Olef_4
1.27E+13 0.00 37.80
C2H3r_Olef+C4H8_Olef_1=C2H4_Olef+C4H7r_Olef_5
2.32E+13 0.00 55.10
C2H3r_Olef+C4H8_Olef_1=C2H4_Olef+C4H7r_Olef_6
2.32E+13 0.00 55.10
C2H3r_Olef+C4H8_Olef_2=C2H4_Olef+C4H7r_Olef_4
1.27E+13 0.00 37.80
C2H3r_Olef+C4H8_Olef_2=C2H4_Olef+C4H7r_Olef_5
2.32E+13 0.00 55.10
C2H3r_Olef+C4H8_Olef_2=C2H4_Olef+C4H7r_Olef_6
2.32E+13 0.00 55.10
C2H3r_Olef+C4H8_Olef_3=C2H4_Olef+C4H7r_Olef_7
2.12E+13 0.00 64.30
C2H3r_Olef+C4H8_Olef_3=C2H4_Olef+C4H7r_Olef_8
1.27E+13 0.00 37.80
C2H3r_Olef+C4H9N=C2H4_Olef+C4H8Nr
6.40E+12 0.00 36.60
C2H3r_Olef+C4H9N=C2H4_Olef+C4H8Nr_1
2.72E+13 0.00 53.90
C2H3r_Olef+C4H9N=C2H4_Olef+C4H8Nr_2
2.72E+13 0.00 53.90
C2H3r_Olef+C4H9N=C2H4_Olef+C4H8Nr_3
1.08E+13 0.00 36.30
C2H3r_Olef+C4H9N=C2H4_Olef+C4H8Nr_Olef_5
6.37E+12 0.00 37.80

C2H3r_Olef+C4H9N_1=C2H4_Olef+C4H8Nr
6.40E+12 0.00 36.60
C2H3r_Olef+C4H9N_1=C2H4_Olef+C4H8Nr_1
2.72E+13 0.00 53.90
C2H3r_Olef+C4H9N_1=C2H4_Olef+C4H8Nr_2
2.72E+13 0.00 53.90
C2H3r_Olef+C4H9N_1=C2H4_Olef+C4H8Nr_3
1.08E+13 0.00 36.30
C2H3r_Olef+C4H9N_1=C2H4_Olef+C4H8Nr_Olef_5
6.37E+12 0.00 37.80
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef
6.40E+12 0.00 36.60
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef_1
2.72E+13 0.00 53.90
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef_2
1.06E+13 0.00 64.30
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef_3
1.06E+13 0.00 64.30
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef_4
1.02E+13 0.00 58.40
C2H3r_Olef+CCNCC=C2H4_Olef+CCjNCC
6.40E+12 0.00 36.60
C2H3r_Olef+CCNCC=C2H4_Olef+CjCNCC
2.72E+13 0.00 53.90
C2H3r_Olef+CH2CHCN=C2H4_Olef+C3H2Nr_Olef
7.97E+12 0.00 44.00
C2H3r_Olef+CH2CHCN=C2H4_Olef+C3H2Nr_Olef_1
1.08E+13 0.00 64.30
C2H3r_Olef+CH2CHCN=C2H4_Olef+C3H2Nr_Olef_2
1.08E+13 0.00 64.30
C2H3r_Olef+CH3CH2CN=C2H4_Olef+C3H4Nr
1.00E+13 0.00 53.90
C2H3r_Olef+CH3CH2CN=C2H4_Olef+C3H4Nr_1
1.00E+13 0.00 33.20
C2H3r_Olef+CH3CN=C2H4_Olef+C2H2Nr
2.16E+13 0.00 40.80
C2H3r_Olef+CH3N=C2H4_Olef+CHNHr
1.23E+13 0.00 41.30
C2H3r_Olef+CH5N=C2H4_Olef+CH4Nr
2.53E+13 0.00 43.40
C2H5r+C2H4_Olef=C2H6+C2H3r_Olef
7.51E+12 0.00 89.70
C2H5r+C2H5N=C2H6+C2H4Nr_2
1.16E+12 0.00 63.30
C2H5r+C2H5N=C2H6+C2H4Nr_3
1.98E+12 0.00 61.80
C2H5r+C2H5N_1=C2H6+C2H4Nr_2
1.16E+12 0.00 63.30
C2H5r+C2H5N_1=C2H6+C2H4Nr_3
1.98E+12 0.00 61.80
C2H5r+C2H5N_2=C2H6+C2H4Nr
2.22E+12 0.00 66.80
C2H5r+C2H5N_2=C2H6+C2H4Nr_1
4.69E+12 0.00 66.00
C2H5r+C2H5N_Olef=C2H6+C2H4Nr_Olef
1.62E+12 0.00 89.80
C2H5r+C2H5N_Olef=C2H6+C2H4Nr_Olef_1
1.62E+12 0.00 89.80

C2H5r+C2H5N_Olef=C2H6+C2H4Nr_Olef_2
1.70E+12 0.00 83.90
C2H5r+C3H5N_Olef=C2H6+C3H4Nr_Olef
1.74E+12 0.00 89.80
C2H5r+C3H5N_Olef=C2H6+C3H4Nr_Olef_1
1.74E+12 0.00 89.80
C2H5r+C3H5N_Olef=C2H6+C3H4Nr_Olef_2
2.25E+12 0.00 66.80
C2H5r+C3H5N_Olef=C2H6+C3H4Nr_Olef_3
1.85E+12 0.00 83.90
C2H5r+C3H6_Olef=C2H6+C3H5r_Olef_1
1.92E+12 0.00 80.60
C2H5r+C3H6_Olef=C2H6+C3H5r_Olef_2
1.70E+12 0.00 89.80
C2H5r+C3H6_Olef=C2H6+C3H5r_Olef_3
1.70E+12 0.00 89.80
C2H5r+C3H7N=C2H6+C3H6Nr_1
1.16E+12 0.00 63.30
C2H5r+C3H7N=C2H6+C3H6Nr_2
1.98E+12 0.00 61.80
C2H5r+C3H7N=C2H6+CH3CHNCH2
4.69E+12 0.00 66.00
C2H5r+C3H7N_1=C2H6+C3H6Nr_1
1.16E+12 0.00 63.30
C2H5r+C3H7N_1=C2H6+C3H6Nr_2
1.98E+12 0.00 61.80
C2H5r+C3H7N_1=C2H6+CH3CHNCH2
4.69E+12 0.00 66.00
C2H5r+C3H7N_2=C2H6+C3H6Nr_3
4.40E+12 0.00 79.10
C2H5r+C3H7N_2=C2H6+C3H6Nr_4
2.25E+12 0.00 66.80
C2H5r+C3H7N_2=C2H6+CH3CHNCH2
1.17E+12 0.00 62.10
C2H5r+C3H7N_Olef=C2H6+C3H6Nr_Olef
1.78E+12 0.00 89.80
C2H5r+C3H7N_Olef=C2H6+C3H6Nr_Olef_1
1.78E+12 0.00 89.80
C2H5r+C3H7N_Olef=C2H6+C3H6Nr_Olef_2
4.61E+12 0.00 68.90
C2H5r+C3H7N_Olef=C2H6+C3H6Nr_Olef_3
1.71E+12 0.00 83.90
C2H5r+C4H5N_Olef=C2H6+C4H4Nr_Olef
1.68E+12 0.00 89.80
C2H5r+C4H5N_Olef=C2H6+C4H4Nr_Olef_1
1.68E+12 0.00 89.80
C2H5r+C4H5N_Olef=C2H6+C4H4Nr_Olef_2
1.02E+12 0.00 59.90
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef
1.87E+12 0.00 89.80
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_1
1.87E+12 0.00 89.80
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_2
1.87E+12 0.00 89.80
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_3
1.87E+12 0.00 89.80
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_4
1.16E+12 0.00 63.30

C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_5
1.85E+12 0.00 83.90
C2H5r+C4H7N_Olef=C2H6+C4H6Nr_Olef_6
1.98E+12 0.00 61.80
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef
1.68E+12 0.00 89.80
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_1
1.68E+12 0.00 89.80
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_2
1.68E+12 0.00 89.80
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_3
1.68E+12 0.00 89.80
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_4
1.16E+12 0.00 63.30
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_5
1.85E+12 0.00 83.90
C2H5r+C4H7N_Olef_1=C2H6+C4H6Nr_Olef_6
1.95E+12 0.00 61.80
C2H5r+C4H8_Olef=C2H6+C4H7r_Olef
4.32E+12 0.00 79.10
C2H5r+C4H8_Olef=C2H6+C4H7r_Olef_1
1.70E+12 0.00 89.80
C2H5r+C4H8_Olef=C2H6+C4H7r_Olef_2
1.70E+12 0.00 89.80
C2H5r+C4H8_Olef=C2H6+C4H7r_Olef_3
1.92E+12 0.00 80.60
C2H5r+C4H8_Olef=C2H6+C4H7r_Olef_4
2.14E+12 0.00 52.90
C2H5r+C4H8_Olef_1=C2H6+C4H7r_Olef_4
2.04E+12 0.00 59.90
C2H5r+C4H8_Olef_1=C2H6+C4H7r_Olef_5
3.84E+12 0.00 80.60
C2H5r+C4H8_Olef_1=C2H6+C4H7r_Olef_6
3.84E+12 0.00 80.60
C2H5r+C4H8_Olef_2=C2H6+C4H7r_Olef_4
2.04E+12 0.00 59.90
C2H5r+C4H8_Olef_2=C2H6+C4H7r_Olef_5
3.81E+12 0.00 80.60
C2H5r+C4H8_Olef_2=C2H6+C4H7r_Olef_6
3.81E+12 0.00 80.60
C2H5r+C4H8_Olef_3=C2H6+C4H7r_Olef_7
3.34E+12 0.00 89.80
C2H5r+C4H8_Olef_3=C2H6+C4H7r_Olef_8
2.04E+12 0.00 59.90
C2H5r+C4H9N=C2H6+C4H8Nr
1.17E+12 0.00 62.10
C2H5r+C4H9N=C2H6+C4H8Nr_1
4.31E+12 0.00 79.10
C2H5r+C4H9N=C2H6+C4H8Nr_2
4.31E+12 0.00 79.10
C2H5r+C4H9N=C2H6+C4H8Nr_3
1.95E+12 0.00 61.80
C2H5r+C4H9N=C2H6+C4H8Nr_Olef_5
1.16E+12 0.00 63.30
C2H5r+C4H9N_1=C2H6+C4H8Nr
1.17E+12 0.00 62.10
C2H5r+C4H9N_1=C2H6+C4H8Nr_1
4.40E+12 0.00 79.10

C2H5r+C4H9N_1=C2H6+C4H8Nr_2
4.40E+12 0.00 79.10
C2H5r+C4H9N_1=C2H6+C4H8Nr_3
1.98E+12 0.00 61.80
C2H5r+C4H9N_1=C2H6+C4H8Nr_Olef_5
1.16E+12 0.00 63.30
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef
1.17E+12 0.00 62.10
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef_1
4.31E+12 0.00 79.10
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef_2
1.68E+12 0.00 89.80
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef_3
1.68E+12 0.00 89.80
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef_4
1.79E+12 0.00 83.90
C2H5r+CCNCC=C2H6+CCjNCC
1.17E+12 0.00 62.10
C2H5r+CCNCC=C2H6+CjCNCC
4.26E+12 0.00 79.10
C2H5r+CH2CHCN=C2H6+C3H2Nr_Olef
1.31E+12 0.00 69.50
C2H5r+CH2CHCN=C2H6+C3H2Nr_Olef_1
1.82E+12 0.00 89.80
C2H5r+CH2CHCN=C2H6+C3H2Nr_Olef_2
1.82E+12 0.00 89.80
C2H5r+CH3CH2CN=C2H6+C3H4Nr
4.40E+12 0.00 79.10
C2H5r+CH3CH2CN=C2H6+C3H4Nr_1
2.59E+12 0.00 58.40
C2H5r+CH3CN=C2H6+C2H2Nr
3.94E+12 0.00 66.30
C2H5r+CH3N=C2H6+CHNHr
2.25E+12 0.00 66.80
C2H5r+CH5N=C2H6+CH4Nr
4.61E+12 0.00 68.90
CH3r+C2H5N=CH4+C2H4Nr_2
7.05E+12 0.00 57.90
CH3r+C2H5N=CH4+C2H4Nr_3
1.20E+13 0.00 56.40
CH3r+C2H5N_1=CH4+C2H4Nr_2
7.05E+12 0.00 57.90
CH3r+C2H5N_1=CH4+C2H4Nr_3
1.20E+13 0.00 56.40
CH3r+C2H5N_Olef=CH4+C2H4Nr_Olef
1.05E+13 0.00 84.40
CH3r+C2H5N_Olef=CH4+C2H4Nr_Olef_1
1.05E+13 0.00 84.40
CH3r+C3H5N_Olef=CH4+C3H4Nr_Olef
1.13E+13 0.00 84.40
CH3r+C3H5N_Olef=CH4+C3H4Nr_Olef_1
1.13E+13 0.00 84.40
CH3r+C3H5N_Olef=CH4+C3H4Nr_Olef_2
1.36E+13 0.00 61.40
CH3r+C3H5N_Olef=CH4+C3H4Nr_Olef_3
1.12E+13 0.00 78.50
CH3r+C3H6_Olef=CH4+C3H5r_Olef
6.95E+12 0.00 58.00

CH3r+C3H6_Olef=CH4+C3H5r_Olef_1
1.25E+13 0.00 75.20
CH3r+C3H6_Olef=CH4+C3H5r_Olef_2
1.10E+13 0.00 84.40
CH3r+C3H6_Olef=CH4+C3H5r_Olef_3
1.10E+13 0.00 84.40
CH3r+C3H7N=CH4+C3H6Nr_1
7.05E+12 0.00 57.90
CH3r+C3H7N=CH4+C3H6Nr_2
1.20E+13 0.00 56.40
CH3r+C3H7N=CH4+CH3CHNCH2
2.84E+13 0.00 60.60
CH3r+C3H7N_1=CH4+C3H6Nr_1
7.05E+12 0.00 57.90
CH3r+C3H7N_1=CH4+C3H6Nr_2
1.20E+13 0.00 56.40
CH3r+C3H7N_1=CH4+CH3CHNCH2
2.84E+13 0.00 60.60
CH3r+C3H7N_2=CH4+C3H6Nr_3
3.00E+13 0.00 74.00
CH3r+C3H7N_2=CH4+C3H6Nr_4
1.36E+13 0.00 61.40
CH3r+C3H7N_2=CH4+CH3CHNCH2
7.08E+12 0.00 56.70
CH3r+C3H7N_Olef=CH4+C3H6Nr_Olef
1.15E+13 0.00 84.40
CH3r+C3H7N_Olef=CH4+C3H6Nr_Olef_1
1.15E+13 0.00 84.40
CH3r+C3H7N_Olef=CH4+C3H6Nr_Olef_2
2.79E+13 0.00 63.50
CH3r+C3H7N_Olef=CH4+C3H6Nr_Olef_3
1.11E+13 0.00 78.50
CH3r+C4H5N_Olef=CH4+C4H4Nr_Olef
1.09E+13 0.00 84.40
CH3r+C4H5N_Olef=CH4+C4H4Nr_Olef_1
1.09E+13 0.00 84.40
CH3r+C4H5N_Olef=CH4+C4H4Nr_Olef_2
7.05E+12 0.00 57.90
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef
1.19E+13 0.00 84.40
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_1
1.19E+13 0.00 84.40
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_2
1.19E+13 0.00 84.40
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_3
1.19E+13 0.00 84.40
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_4
7.05E+12 0.00 57.90
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_5
1.12E+13 0.00 78.50
CH3r+C4H7N_Olef=CH4+C4H6Nr_Olef_6
1.20E+13 0.00 56.40
CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef
1.09E+13 0.00 84.40
CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_1
1.09E+13 0.00 84.40
CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_2
1.09E+13 0.00 84.40

CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_3
 1.09E+13 0.00 84.40
 CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_4
 7.05E+12 0.00 57.90
 CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_5
 1.12E+13 0.00 78.50
 CH3r+C4H7N_Olef_1=CH4+C4H6Nr_Olef_6
 1.20E+13 0.00 56.40
 CH3r+C4H8_Olef=CH4+C4H7r_Olef
 3.00E+13 0.00 74.00
 CH3r+C4H8_Olef=CH4+C4H7r_Olef_1
 1.10E+13 0.00 84.40
 CH3r+C4H8_Olef=CH4+C4H7r_Olef_2
 1.10E+13 0.00 84.40
 CH3r+C4H8_Olef=CH4+C4H7r_Olef_3
 1.24E+13 0.00 75.20
 CH3r+C4H8_Olef=CH4+C4H7r_Olef_4
 1.45E+13 0.00 50.90
 CH3r+C4H8_Olef_1=CH4+C4H7r_Olef_4
 1.41E+13 0.00 57.90
 CH3r+C4H8_Olef_1=CH4+C4H7r_Olef_5
 2.49E+13 0.00 75.20
 CH3r+C4H8_Olef_1=CH4+C4H7r_Olef_6
 2.49E+13 0.00 75.20
 CH3r+C4H8_Olef_2=CH4+C4H7r_Olef_4
 1.41E+13 0.00 57.90
 CH3r+C4H8_Olef_2=CH4+C4H7r_Olef_5
 2.47E+13 0.00 75.20
 CH3r+C4H8_Olef_2=CH4+C4H7r_Olef_6
 2.47E+13 0.00 75.20
 CH3r+C4H8_Olef_3=CH4+C4H7r_Olef_7
 2.17E+13 0.00 84.40
 CH3r+C4H8_Olef_3=CH4+C4H7r_Olef_8
 1.41E+13 0.00 57.90
 CH3r+C4H9N=CH4+C4H8Nr
 7.08E+12 0.00 56.70
 CH3r+C4H9N=CH4+C4H8Nr_1
 3.00E+13 0.00 74.00
 CH3r+C4H9N=CH4+C4H8Nr_2
 3.00E+13 0.00 74.00
 CH3r+C4H9N=CH4+C4H8Nr_3
 1.20E+13 0.00 56.40
 CH3r+C4H9N=CH4+C4H8Nr_Olef_5
 7.05E+12 0.00 57.90
 CH3r+C4H9N_1=CH4+C4H8Nr
 7.08E+12 0.00 56.70
 CH3r+C4H9N_1=CH4+C4H8Nr_1
 3.00E+13 0.00 74.00
 CH3r+C4H9N_1=CH4+C4H8Nr_2
 3.00E+13 0.00 74.00
 CH3r+C4H9N_1=CH4+C4H8Nr_3
 1.20E+13 0.00 56.40
 CH3r+C4H9N_1=CH4+C4H8Nr_Olef_5
 7.05E+12 0.00 57.90
 CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef
 7.08E+12 0.00 56.70
 CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef_1
 3.00E+13 0.00 74.00

CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef_2
 1.09E+13 0.00 84.40
 CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef_3
 1.09E+13 0.00 84.40
 CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef_4
 1.12E+13 0.00 78.50
 CH3r+CCNCC=CH4+CCjNCC
 3.52E+12 0.00 32.7
 CH3r+CCNCC=CH4+CjCNCC
 5.58E-09 6.567 17.909
 CH3r+CH2CHCN=CH4+C3H2Nr_Olef
 8.49E+12 0.00 64.10
 CH3r+CH2CHCN=CH4+C3H2Nr_Olef_1
 1.17E+13 0.00 84.40
 CH3r+CH2CHCN=CH4+C3H2Nr_Olef_2
 1.17E+13 0.00 84.40
 CH3r+CH3CH2CN=CH4+C3H4Nr
 3.00E+13 0.00 74.00
 CH3r+CH3CH2CN=CH4+C3H4Nr_1
 7.50E+12 0.00 53.30
 CH4Nr+C2H5N=CH5N+C2H4Nr_2
 1.16E+13 0.00 87.10
 CH4Nr+C2H5N=CH5N+C2H4Nr_3
 1.81E+13 0.00 85.60
 CH4Nr+C2H5N_1=CH5N+C2H4Nr_2
 1.16E+13 0.00 87.10
 CH4Nr+C2H5N_1=CH5N+C2H4Nr_3
 1.81E+13 0.00 85.60
 CH4Nr+C2H5N_2=CH5N+C2H4Nr
 2.01E+13 0.00 90.60
 CH4Nr+C2H5N_2=CH5N+C2H4Nr_1
 4.65E+13 0.00 89.80
 CH4Nr+C2H5N_Olef=CH5N+C2H4Nr_Olef
 1.47E+13 0.00 113.60
 CH4Nr+C2H5N_Olef=CH5N+C2H4Nr_Olef_1
 1.47E+13 0.00 113.60
 CH4Nr+C2H5N_Olef=CH5N+C2H4Nr_Olef_2
 1.54E+13 0.00 107.70
 CH4Nr+C3H5N_Olef=CH5N+C3H4Nr_Olef
 1.58E+13 0.00 113.60
 CH4Nr+C3H5N_Olef=CH5N+C3H4Nr_Olef_1
 1.58E+13 0.00 113.60
 CH4Nr+C3H5N_Olef=CH5N+C3H4Nr_Olef_2
 2.24E+13 0.00 90.60
 CH4Nr+C3H5N_Olef=CH5N+C3H4Nr_Olef_3
 1.83E+13 0.00 107.70
 CH4Nr+C3H6_Olef=CH5N+C3H5r_Olef
 1.16E+13 0.00 87.10
 CH4Nr+C3H6_Olef=CH5N+C3H5r_Olef_1
 1.74E+13 0.00 104.40
 CH4Nr+C3H6_Olef=CH5N+C3H5r_Olef_2
 1.54E+13 0.00 113.60
 CH4Nr+C3H6_Olef=CH5N+C3H5r_Olef_3
 1.54E+13 0.00 113.60
 CH4Nr+C3H7N=CH5N+C3H6Nr_1
 1.16E+13 0.00 87.10
 CH4Nr+C3H7N=CH5N+C3H6Nr_2
 1.96E+13 0.00 85.60

CH4Nr+C3H7N=CH5N+CH3CHNCH2
4.65E+13 0.00 89.80
CH4Nr+C3H7N_1=CH5N+C3H6Nr_1
1.16E+13 0.00 87.10
CH4Nr+C3H7N_1=CH5N+C3H6Nr_2
1.88E+13 0.00 85.60
CH4Nr+C3H7N_1=CH5N+CH3CHNCH2
4.65E+13 0.00 89.80
CH4Nr+C3H7N_2=CH5N+C3H6Nr_3
4.90E+13 0.00 103.20
CH4Nr+C3H7N_2=CH5N+C3H6Nr_4
2.24E+13 0.00 90.60
CH4Nr+C3H7N_2=CH5N+CH3CHNCH2
1.16E+13 0.00 85.90
CH4Nr+C3H7N_Olef=CH5N+C3H6Nr_Olef
1.61E+13 0.00 113.60
CH4Nr+C3H7N_Olef=CH5N+C3H6Nr_Olef_1
1.61E+13 0.00 113.60
CH4Nr+C3H7N_Olef=CH5N+C3H6Nr_Olef_2
4.58E+13 0.00 92.70
CH4Nr+C3H7N_Olef=CH5N+C3H6Nr_Olef_3
1.55E+13 0.00 107.70
CH4Nr+C4H5N_Olef=CH5N+C4H4Nr_Olef
1.52E+13 0.00 113.60
CH4Nr+C4H5N_Olef=CH5N+C4H4Nr_Olef_1
1.52E+13 0.00 113.60
CH4Nr+C4H5N_Olef=CH5N+C4H4Nr_Olef_2
1.16E+13 0.00 87.10
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef
1.69E+13 0.00 113.60
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_1
1.69E+13 0.00 113.60
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_2
1.69E+13 0.00 113.60
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_3
1.69E+13 0.00 113.60
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_4
1.16E+13 0.00 87.10
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_5
1.83E+13 0.00 107.70
CH4Nr+C4H7N_Olef=CH5N+C4H6Nr_Olef_6
1.96E+13 0.00 85.60
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef
1.52E+13 0.00 113.60
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_1
1.52E+13 0.00 113.60
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_2
1.52E+13 0.00 113.60
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_3
1.52E+13 0.00 113.60
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_4
1.16E+13 0.00 87.10
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_5
1.79E+13 0.00 107.70
CH4Nr+C4H7N_Olef_1=CH5N+C4H6Nr_Olef_6
1.77E+13 0.00 85.60
CH4Nr+C4H8_Olef=CH5N+C4H7r_Olef
4.41E+13 0.00 103.20

CH4Nr+C4H8_Olef=CH5N+C4H7r_Olef_1
1.54E+13 0.00 113.60
CH4Nr+C4H8_Olef=CH5N+C4H7r_Olef_2
1.54E+13 0.00 113.60
CH4Nr+C4H8_Olef=CH5N+C4H7r_Olef_3
1.74E+13 0.00 104.40
CH4Nr+C4H8_Olef=CH5N+C4H7r_Olef_4
2.44E+13 0.00 80.10
CH4Nr+C4H8_Olef_1=CH5N+C4H7r_Olef_4
2.31E+13 0.00 87.10
CH4Nr+C4H8_Olef_1=CH5N+C4H7r_Olef_5
3.48E+13 0.00 104.40
CH4Nr+C4H8_Olef_1=CH5N+C4H7r_Olef_6
3.48E+13 0.00 104.40
CH4Nr+C4H8_Olef_2=CH5N+C4H7r_Olef_4
2.31E+13 0.00 87.10
CH4Nr+C4H8_Olef_2=CH5N+C4H7r_Olef_5
3.46E+13 0.00 104.40
CH4Nr+C4H8_Olef_2=CH5N+C4H7r_Olef_6
3.46E+13 0.00 104.40
CH4Nr+C4H8_Olef_3=CH5N+C4H7r_Olef_7
3.03E+13 0.00 113.60
CH4Nr+C4H8_Olef_3=CH5N+C4H7r_Olef_8
2.31E+13 0.00 87.10
CH4Nr+C4H9N=CH5N+C4H8Nr
1.15E+13 0.00 85.90
CH4Nr+C4H9N=CH5N+C4H8Nr_1
4.40E+13 0.00 103.20
CH4Nr+C4H9N=CH5N+C4H8Nr_2
4.40E+13 0.00 103.20
CH4Nr+C4H9N=CH5N+C4H8Nr_3
1.77E+13 0.00 85.60
CH4Nr+C4H9N=CH5N+C4H8Nr_Olef_5
1.16E+13 0.00 87.10
CH4Nr+C4H9N_1=CH5N+C4H8Nr
1.16E+13 0.00 85.90
CH4Nr+C4H9N_1=CH5N+C4H8Nr_1
4.90E+13 0.00 103.20
CH4Nr+C4H9N_1=CH5N+C4H8Nr_2
4.90E+13 0.00 103.20
CH4Nr+C4H9N_1=CH5N+C4H8Nr_3
1.97E+13 0.00 85.60
CH4Nr+C4H9N_1=CH5N+C4H8Nr_Olef_5
1.16E+13 0.00 87.10
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef
1.16E+13 0.00 85.90
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef_1
4.40E+13 0.00 103.20
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef_2
1.52E+13 0.00 113.60
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef_3
1.52E+13 0.00 113.60
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef_4
1.62E+13 0.00 107.70
CH4Nr+CCNCC=CH5N+CCjNCC
1.16E+13 0.00 85.90
CH4Nr+CCNCC=CH5N+CjCNCC
4.36E+13 0.00 103.20

CH4Nr+CH2CHCN=CH5N+C3H2Nr_Olef
 1.19E+13 0.00 93.30
 CH4Nr+CH2CHCN=CH5N+C3H2Nr_Olef_1
 1.65E+13 0.00 113.60
 CH4Nr+CH2CHCN=CH5N+C3H2Nr_Olef_2
 1.65E+13 0.00 113.60
 CH4Nr+CH3CH2CN=CH5N+C3H4Nr
 4.90E+13 0.00 103.20
 CH4Nr+CH3CH2CN=CH5N+C3H4Nr_1
 2.90E+13 0.00 82.50
 CH4Nr+CH3CN=CH5N+C2H2Nr
 3.79E+13 0.00 90.10
 CH4Nr+CH3N=CH5N+CHNHr
 2.17E+13 0.00 90.60
 CHNHr+C2H5N=CH3N+C2H4Nr_2
 1.13E+13 0.00 75.20
 CHNHr+C2H5N=CH3N+C2H4Nr_3
 1.83E+13 0.00 73.70
 CHNHr+C2H5N_1=CH3N+C2H4Nr_2
 1.13E+13 0.00 75.20
 CHNHr+C2H5N_1=CH3N+C2H4Nr_3
 1.83E+13 0.00 73.70
 CHNHr+C2H5N_2=CH3N+C2H4Nr
 2.04E+13 0.00 78.70
 CHNHr+C2H5N_2=CH3N+C2H4Nr_1
 4.57E+13 0.00 77.90
 CHNHr+C2H5N_Olef=CH3N+C2H4Nr_Olef
 1.48E+13 0.00 101.70
 CHNHr+C2H5N_Olef=CH3N+C2H4Nr_Olef_1
 1.48E+13 0.00 101.70
 CHNHr+C2H5N_Olef=CH3N+C2H4Nr_Olef_2
 1.56E+13 0.00 95.80
 CHNHr+C3H5N_Olef=CH3N+C3H4Nr_Olef
 1.60E+13 0.00 101.70
 CHNHr+C3H5N_Olef=CH3N+C3H4Nr_Olef_1
 1.60E+13 0.00 101.70
 CHNHr+C3H5N_Olef=CH3N+C3H4Nr_Olef_2
 2.20E+13 0.00 78.70
 CHNHr+C3H5N_Olef=CH3N+C3H4Nr_Olef_3
 1.80E+13 0.00 95.80
 CHNHr+C3H6_Olef=CH3N+C3H5r_Olef
 1.13E+13 0.00 75.20
 CHNHr+C3H6_Olef=CH3N+C3H5r_Olef_1
 1.76E+13 0.00 92.50
 CHNHr+C3H6_Olef=CH3N+C3H5r_Olef_2
 1.56E+13 0.00 101.70
 CHNHr+C3H6_Olef=CH3N+C3H5r_Olef_3
 1.56E+13 0.00 101.70
 CHNHr+C3H7N=CH3N+C3H6Nr_1
 1.13E+13 0.00 75.20
 CHNHr+C3H7N=CH3N+C3H6Nr_2
 1.93E+13 0.00 73.70
 CHNHr+C3H7N=CH3N+CH3CHNCH2
 4.57E+13 0.00 77.90
 CHNHr+C3H7N_1=CH3N+C3H6Nr_1
 1.13E+13 0.00 75.20
 CHNHr+C3H7N_1=CH3N+C3H6Nr_2
 1.90E+13 0.00 73.70

CHNHr+C3H7N_1=CH3N+CH3CHNCH2
4.57E+13 0.00 77.90
CHNHr+C3H7N_2=CH3N+C3H6Nr_3
4.82E+13 0.00 91.30
CHNHr+C3H7N_2=CH3N+C3H6Nr_4
2.20E+13 0.00 78.70
CHNHr+C3H7N_2=CH3N+CH3CHNCH2
1.14E+13 0.00 74.00
CHNHr+C3H7N_Olef=CH3N+C3H6Nr_Olef
1.63E+13 0.00 101.70
CHNHr+C3H7N_Olef=CH3N+C3H6Nr_Olef_1
1.63E+13 0.00 101.70
CHNHr+C3H7N_Olef=CH3N+C3H6Nr_Olef_2
4.49E+13 0.00 80.80
CHNHr+C3H7N_Olef=CH3N+C3H6Nr_Olef_3
1.57E+13 0.00 95.80
CHNHr+C4H5N_Olef=CH3N+C4H4Nr_Olef
1.54E+13 0.00 101.70
CHNHr+C4H5N_Olef=CH3N+C4H4Nr_Olef_1
1.54E+13 0.00 101.70
CHNHr+C4H5N_Olef=CH3N+C4H4Nr_Olef_2
1.13E+13 0.00 75.20
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef
1.71E+13 0.00 101.70
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_1
1.71E+13 0.00 101.70
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_2
1.71E+13 0.00 101.70
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_3
1.71E+13 0.00 101.70
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_4
1.13E+13 0.00 75.20
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_5
1.80E+13 0.00 95.80
CHNHr+C4H7N_Olef=CH3N+C4H6Nr_Olef_6
1.93E+13 0.00 73.70
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef
1.54E+13 0.00 101.70
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_1
1.54E+13 0.00 101.70
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_2
1.54E+13 0.00 101.70
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_3
1.54E+13 0.00 101.70
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_4
1.13E+13 0.00 75.20
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_5
1.80E+13 0.00 95.80
CHNHr+C4H7N_Olef_1=CH3N+C4H6Nr_Olef_6
1.79E+13 0.00 73.70
CHNHr+C4H8_Olef=CH3N+C4H7r_Olef
4.46E+13 0.00 91.30
CHNHr+C4H8_Olef=CH3N+C4H7r_Olef_1
1.55E+13 0.00 101.70
CHNHr+C4H8_Olef=CH3N+C4H7r_Olef_2
1.55E+13 0.00 101.70
CHNHr+C4H8_Olef=CH3N+C4H7r_Olef_3
1.76E+13 0.00 92.50

CHNHr+C4H8_Olef=CH3N+C4H7r_Olef_4
 2.39E+13 0.00 68.20
 CHNHr+C4H8_Olef_1=CH3N+C4H7r_Olef_4
 2.27E+13 0.00 75.20
 CHNHr+C4H8_Olef_1=CH3N+C4H7r_Olef_5
 3.52E+13 0.00 92.50
 CHNHr+C4H8_Olef_1=CH3N+C4H7r_Olef_6
 3.52E+13 0.00 92.50
 CHNHr+C4H8_Olef_2=CH3N+C4H7r_Olef_4
 2.27E+13 0.00 75.20
 CHNHr+C4H8_Olef_2=CH3N+C4H7r_Olef_5
 3.49E+13 0.00 92.50
 CHNHr+C4H8_Olef_2=CH3N+C4H7r_Olef_6
 3.49E+13 0.00 92.50
 CHNHr+C4H8_Olef_3=CH3N+C4H7r_Olef_7
 3.06E+13 0.00 101.70
 CHNHr+C4H8_Olef_3=CH3N+C4H7r_Olef_8
 2.27E+13 0.00 75.20
 CHNHr+C4H9N=CH3N+C4H8Nr
 1.14E+13 0.00 74.00
 CHNHr+C4H9N=CH3N+C4H8Nr_1
 4.45E+13 0.00 91.30
 CHNHr+C4H9N=CH3N+C4H8Nr_2
 4.45E+13 0.00 91.30
 CHNHr+C4H9N=CH3N+C4H8Nr_3
 1.79E+13 0.00 73.70
 CHNHr+C4H9N=CH3N+C4H8Nr_Olef_5
 1.13E+13 0.00 75.20
 CHNHr+C4H9N_1=CH3N+C4H8Nr
 1.14E+13 0.00 74.00
 CHNHr+C4H9N_1=CH3N+C4H8Nr_1
 4.82E+13 0.00 91.30
 CHNHr+C4H9N_1=CH3N+C4H8Nr_2
 4.82E+13 0.00 91.30
 CHNHr+C4H9N_1=CH3N+C4H8Nr_3
 1.93E+13 0.00 73.70
 CHNHr+C4H9N_1=CH3N+C4H8Nr_Olef_5
 1.13E+13 0.00 75.20
 CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef
 1.14E+13 0.00 74.00
 CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef_1
 4.45E+13 0.00 91.30
 CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef_2
 1.54E+13 0.00 101.70
 CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef_3
 1.54E+13 0.00 101.70
 CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef_4
 1.64E+13 0.00 95.80
 CHNHr+CCNCC=CH3N+CCjNCC
 1.14E+13 0.00 74.00
 CHNHr+CCNCC=CH3N+CjCNCC
 4.40E+13 0.00 91.30
 CHNHr+CH2CHCN=CH3N+C3H2Nr_Olef
 1.20E+13 0.00 81.40
 CHNHr+CH2CHCN=CH3N+C3H2Nr_Olef_1
 1.67E+13 0.00 101.70
 CHNHr+CH2CHCN=CH3N+C3H2Nr_Olef_2
 1.67E+13 0.00 101.70

CHNHr+CH3CH2CN=CH3N+C3H4Nr	4.82E+13	0.00	91.30	
CHNHr+CH3CH2CN=CH3N+C3H4Nr_1	2.84E+13	0.00	70.60	
CHNHr+CH3CN=CH3N+C2H2Nr	3.83E+13	0.00	78.20	
C4H8Nr=C4H8Nr_3	1.30E+45	-10.07		276.60
CH3CHNCH2=C3H6Nr_2	1.30E+45	-10.07		276.60
C2H5r+C3H8=C2H6+C3H7r	3.05E12	0.000	69.5	
C3H5r_Olef+C2H6=C3H6_Olef+C2H5r	1.06E14	0.000	121.6	
C3H5r_Olef+C3H8=C3H6_Olef+C3H7r	3.59E13	0.000	107.9	
C3H5r_Olef+C3H8=C3H6_Olef+C3H7r_1	0.000	121.9		1.12E14
C3H7r_1+C2H6=C3H8+C2H5r	8.80E12	0.000	79.1	
C3H7r_1+C3H8=C3H8+C3H7r	3.05E12	0.000	69.5	
CH3r+C2H6=CH4+C2H5r	5.84E13	0.000	74.0	
CH3r+C3H8=CH4+C3H7r_1	2.05E13	0.000	64.4	
CH3r+C3H8=CH4+C3H7r	1.50E3	2.960	46.0	
Hr+C2H5N=H2+C2H4Nr_2	7.64E+13	0.00	38.40	
Hr+C2H5N=H2+C2H4Nr_3	1.33E+14	0.00	35.70	
Hr+C2H5N_1=H2+C2H4Nr_2	7.64E+13	0.00	38.40	
Hr+C2H5N_1=H2+C2H4Nr_3	1.33E+14	0.00	35.70	
Hr+C2H5N_Olef=H2+C2H4Nr_Olef	1.81E+14	0.00	72.10	
Hr+C2H5N_Olef=H2+C2H4Nr_Olef_1	1.81E+14	0.00	72.10	
Hr+C3H5N_Olef=H2+C3H4Nr_Olef	1.98E+14	0.00	72.10	
Hr+C3H5N_Olef=H2+C3H4Nr_Olef_1	1.98E+14	0.00	72.10	
Hr+C3H5N_Olef=H2+C3H4Nr_Olef_2	1.42E+14	0.00	42.70	
Hr+C3H5N_Olef=H2+C3H4Nr_Olef_3	5.10E+13	0.00	65.90	
Hr+C3H6_Olef=H2+C3H5r_Olef	8.30E+13	0.00	38.40	
!!Hr+C3H6_Olef=H2+C3H5r_Olef_1	1.99E+14	0.00	60.00	
Hr+C3H6_Olef=H2+C3H5r_Olef_1	3.00E+07	1.97	54.80	
Hr+C3H6_Olef=H2+C3H5r_Olef_2	1.93E+14	0.00	72.10	
Hr+C3H6_Olef=H2+C3H5r_Olef_3	1.93E+14	0.00	72.10	

Hr+C3H7N=H2+C3H6Nr_1
 7.64E+13 0.00 38.40
 Hr+C3H7N=H2+C3H6Nr_2
 1.33E+14 0.00 35.70
 Hr+C3H7N=H2+CH3CHNCH2
 1.46E+14 0.00 45.60
 Hr+C3H7N_1=H2+C3H6Nr_1
 7.64E+13 0.00 38.40
 Hr+C3H7N_1=H2+C3H6Nr_2
 1.33E+14 0.00 35.70
 Hr+C3H7N_1=H2+CH3CHNCH2
 1.46E+14 0.00 45.60
 Hr+C3H7N_2=H2+C3H6Nr_3
 3.89E+14 0.00 53.50
 Hr+C3H7N_2=H2+C3H6Nr_4
 1.42E+14 0.00 42.70
 Hr+C3H7N_2=H2+CH3CHNCH2
 9.72E+13 0.00 45.60
 Hr+C3H7N_Olef=H2+C3H6Nr_Olef
 2.00E+14 0.00 72.10
 Hr+C3H7N_Olef=H2+C3H6Nr_Olef_1
 2.00E+14 0.00 72.10
 Hr+C3H7N_Olef=H2+C3H6Nr_Olef_2
 1.56E+14 0.00 36.20
 Hr+C3H7N_Olef=H2+C3H6Nr_Olef_3
 5.05E+13 0.00 65.90
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef
 2.04E+14 0.00 72.10
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_1
 2.04E+14 0.00 72.10
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_2
 2.04E+14 0.00 72.10
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_3
 2.04E+14 0.00 72.10
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_4
 7.64E+13 0.00 38.40
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_5
 5.10E+13 0.00 65.90
 Hr+C4H7N_Olef=H2+C4H6Nr_Olef_6
 1.33E+14 0.00 35.70
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef
 1.90E+14 0.00 72.10
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_1
 1.90E+14 0.00 72.10
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_2
 1.90E+14 0.00 72.10
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_3
 1.90E+14 0.00 72.10
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_4
 7.64E+13 0.00 38.40
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_5
 5.10E+13 0.00 65.90
 Hr+C4H7N_Olef_1=H2+C4H6Nr_Olef_6
 1.33E+14 0.00 35.70
 Hr+C4H8_Olef=H2+C4H7r_Olef
 3.89E+14 0.00 53.50
 Hr+C4H8_Olef=H2+C4H7r_Olef_1
 1.93E+14 0.00 72.10

Hr+C4H8_Olef=H2+C4H7r_Olef_2
 1.93E+14 0.00 72.10
 Hr+C4H8_Olef=H2+C4H7r_Olef_3
 1.94E+14 0.00 60.00
 Hr+C4H8_Olef=H2+C4H7r_Olef_4
 1.70E+14 0.00 30.80
 Hr+C4H8_Olef_1=H2+C4H7r_Olef_4
 1.53E+14 0.00 38.40
 Hr+C4H8_Olef_1=H2+C4H7r_Olef_5
 3.89E+14 0.00 60.00
 Hr+C4H8_Olef_1=H2+C4H7r_Olef_6
 3.89E+14 0.00 60.00
 Hr+C4H8_Olef_2=H2+C4H7r_Olef_4
 1.53E+14 0.00 38.40
 Hr+C4H8_Olef_2=H2+C4H7r_Olef_5
 3.86E+14 0.00 60.00
 Hr+C4H8_Olef_2=H2+C4H7r_Olef_6
 3.86E+14 0.00 60.00
 Hr+C4H8_Olef_3=H2+C4H7r_Olef_7
 3.78E+14 0.00 72.10
 Hr+C4H8_Olef_3=H2+C4H7r_Olef_8
 1.53E+14 0.00 38.40
 Hr+C4H9N=H2+C4H8Nr
 9.72E+13 0.00 45.60
 Hr+C4H9N=H2+C4H8Nr_1
 3.89E+14 0.00 53.50
 Hr+C4H9N=H2+C4H8Nr_2
 3.89E+14 0.00 53.50
 Hr+C4H9N=H2+C4H8Nr_3
 1.33E+14 0.00 35.70
 Hr+C4H9N=H2+C4H8Nr_Olef_5
 7.64E+13 0.00 38.40
 Hr+C4H9N_1=H2+C4H8Nr
 9.72E+13 0.00 45.60
 Hr+C4H9N_1=H2+C4H8Nr_1
 3.89E+14 0.00 53.50
 Hr+C4H9N_1=H2+C4H8Nr_2
 3.89E+14 0.00 53.50
 Hr+C4H9N_1=H2+C4H8Nr_3
 1.33E+14 0.00 35.70
 Hr+C4H9N_1=H2+C4H8Nr_Olef_5
 7.64E+13 0.00 38.40
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef
 1.04E+14 0.00 36.20
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef_1
 3.89E+14 0.00 53.50
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef_2
 1.90E+14 0.00 72.10
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef_3
 1.90E+14 0.00 72.10
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef_4
 5.10E+13 0.00 65.90
 Hr+CCNCC=H2+CCjNCC
 2.04E+14 0.00 36.20
 Hr+CCNCC=H2+CjCNCC
 3.89E+14 0.00 53.50
 Hr+C2H6=H2+C2H5r
 0.00 53.50

8.09E14

Hr+C3H8=H2+C3H7r_1
2.78E14 0.00 42.40
Hr+C3H8=H2+C3H7r
8.00E+07 1.99 33.90

!! Reaction Family: h abstractions C* + H-N
C2H3r_Olef+C2H5N_Olef=C2H4_Olef+C2H4Nr_2
9.20E+11 0.00 57.80
C2H3r_Olef+C3H7N_Olef=C2H4_Olef+C3H6Nr_1
1.09E+12 0.00 51.00
C2H3r_Olef+C4H9N_Olef=C2H4_Olef+C4H8Nr_Olef_5
1.09E+12 0.00 51.00
C2H3r_Olef+CCNCC=C2H4_Olef+CCNjCC
2.67E+12 0.00 47.70
C2H3r_Olef+CH5N=C2H4_Olef+CH4Nr_1
1.86E+12 0.00 60.80
C2H5r+C2H5N_Olef=C2H6+C2H4Nr_2
1.84E+12 0.00 57.80
C2H5r+C3H7N_Olef=C2H6+C3H6Nr_1
2.18E+12 0.00 51.00
C2H5r+C4H9N_Olef=C2H6+C4H8Nr_Olef_5
2.18E+12 0.00 51.00
C2H5r+CCNCC=C2H6+CCNjCC
1.00E+13 0.00 47.70
C2H5r+CH5N=C2H6+CH4Nr_1
3.71E+12 0.00 60.80
CH3r+C3H7N_Olef=CH4+C3H6Nr_1
2.18E+12 0.00 51.00
CH3r+C4H9N_Olef=CH4+C4H8Nr_Olef_5
2.18E+12 0.00 51.00
CH3r+CCNCC=CH4+CCNjCC
8.11E+11 0.00 29.80
CH4Nr+C2H5N_Olef=CH5N+C2H4Nr_2
1.84E+12 0.00 57.80
CH4Nr+C3H7N_Olef=CH5N+C3H6Nr_1
2.18E+12 0.00 51.00
CH4Nr+C4H9N_Olef=CH5N+C4H8Nr_Olef_5
2.18E+12 0.00 51.00
CH4Nr+CCNCC=CH5N+CCNjCC
5.34E+12 0.00 47.70
CH4Nr+CH5N=CH5N+CH4Nr_1
3.45E+12 0.00 60.80
CHNHr+C2H5N_Olef=CH3N+C2H4Nr_2
9.20E+11 0.00 57.80
CHNHr+C3H7N_Olef=CH3N+C3H6Nr_1
1.09E+12 0.00 51.00
CHNHr+C4H9N_Olef=CH3N+C4H8Nr_Olef_5
1.09E+12 0.00 51.00
CHNHr+CCNCC=CH3N+CCNjCC
2.67E+12 0.00 47.70
CHNHr+CH5N=CH3N+CH4Nr_1
1.77E+12 0.00 60.80

!! Reaction Family: h abstractions N* + H-N
CH2Nr+C2H5N=CH3N+C2H4Nr_4
2.78E+13 0.00 78.10
CH2Nr+C2H5N_1=CH3N+C2H4Nr_4
2.78E+13 0.00 78.10

CH2Nr+C2H5N_Olef=CH3N+C2H4Nr_2
 1.06E+13 0.00 83.50
 CH2Nr+C3H7N_Olef=CH3N+C3H6Nr_1
 2.28E+13 0.00 83.40
 CH2Nr+C4H9N_Olef=CH3N+C4H8Nr_Olef_5
 2.28E+13 0.00 83.40
 CH2Nr+CCNCC=CH3N+CCNjCC
 2.17E+13 0.00 83.40
 CH4Nr_1+C2H5N=CH5N+C2H4Nr_4
 2.64E+12 0.00 46.20
 CH4Nr_1+C2H5N_1=CH5N+C2H4Nr_4
 2.64E+12 0.00 46.20
 CH4Nr_1+C2H5N_Olef=CH5N+C2H4Nr_2
 9.97E+11 0.00 51.60
 CH4Nr_1+C3H7N_Olef=CH5N+C3H6Nr_1
 2.13E+12 0.00 51.50
 CH4Nr_1+C4H9N_Olef=CH5N+C4H8Nr_Olef_5
 2.13E+12 0.00 51.50
 CH4Nr_1+CCNCC=CH5N+CCNjCC
 2.13E+12 0.00 51.50
 CH4Nr_1+CH3N=CH5N+CH2Nr
 2.64E+12 0.00 46.20
 H2Nr+C2H5N=H3N+C2H4Nr_4
 7.82E+12 0.00 27.70
 H2Nr+C2H5N_1=H3N+C2H4Nr_4
 7.82E+12 0.00 27.70
 H2Nr+C3H7N_Olef=H3N+C3H6Nr_1
 6.30E+12 0.00 33.00
 H2Nr+C4H9N_Olef=H3N+C4H8Nr_Olef_5
 6.30E+12 0.00 33.00
 H2Nr+CCNCC=H3N+CCNjCC
 6.30E+12 0.00 33.00
 HO+r+C3H7N=H2O+CH3CHNCH2
 4.20E+13 0.00 0.00
 HO+r+C3H7N_1=H2O+CH3CHNCH2
 4.20E+13 0.00 0.00
 HO+r+C3H7N_2=H2O+CH3CHNCH2
 2.80E+13 0.00 0.00
 HO+r+C3H7N_Olef=H2O+C3H6Nr_Olef_2
 4.20E+13 0.00 0.00
 HO+r+C4H9N=H2O+C4H8Nr
 2.80E+13 0.00 0.00
 HO+r+C4H9N_1=H2O+C4H8Nr
 2.80E+13 0.00 0.00
 HO+r+C4H9N_Olef=H2O+C4H8Nr_Olef
 2.80E+13 0.00 0.00

!! Reaction Family: h abstractions OH* + CH3 - Sivaramakrishnan and Michael 2009

HO+r+C2H5N=H2O+C2H4Nr_2
 1.36E+07 1.81 3.10
 HO+r+C2H5N_1=H2O+C2H4Nr_2
 1.36E+07 1.81 3.10
 HO+r+C3H6_Olef=H2O+C3H5r_Olef
 1.36E+07 1.81 3.10
 HO+r+C3H7N=H2O+C3H6Nr_1
 1.36E+07 1.81 3.10

HOr+C3H7N_1=H2O+C3H6Nr_1
 1.36E+07 1.81 3.10
 HOr+C3H7N_2=H2O+C3H6Nr_3
 1.36E+07 1.81 3.10
 HOr+C4H5N_Olef=H2O+C4H4Nr_Olef_2
 1.36E+07 1.81 3.10
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_4
 1.36E+07 1.81 3.10
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_4
 1.36E+07 1.81 3.10
 HOr+C4H8_Olef=H2O+C4H7r_Olef
 1.36E+07 1.81 3.10
 HOr+C4H8_Olef_1=H2O+C4H7r_Olef_4
 2.73E+07 1.81 3.10
 HOr+C4H8_Olef_2=H2O+C4H7r_Olef_4
 2.73E+07 1.81 3.10
 HOr+C4H8_Olef_3=H2O+C4H7r_Olef_8
 2.73E+07 1.81 3.10
 HOr+C4H9N=H2O+C4H8Nr_1
 1.36E+07 1.81 3.10
 HOr+C4H9N=H2O+C4H8Nr_2
 1.36E+07 1.81 3.10
 HOr+C4H9N=H2O+C4H8Nr_Olef_5
 1.36E+07 1.81 3.10
 HOr+C4H9N_1=H2O+C4H8Nr_1
 1.36E+07 1.81 3.10
 HOr+C4H9N_1=H2O+C4H8Nr_2
 1.36E+07 1.81 3.10
 HOr+C4H9N_1=H2O+C4H8Nr_Olef_5
 1.36E+07 1.81 3.10
 HOr+C4H9N_Olef=H2O+C4H8Nr_Olef_1
 1.36E+07 1.81 3.10
 HOr+CH3CH2CN=H2O+C3H4Nr
 1.36E+07 1.81 3.10

!! Reaction Family: h abstractions OH* + H-N - Lucassen et al.

HOr+C2H5N=H2O+C2H4Nr_4
 1.360E+07 1.813 3.10
 HOr+C2H5N_1=H2O+C2H4Nr_4
 1.360E+07 1.813 3.10
 HOr+C3H7N_Olef=H2O+C3H6Nr_1
 5.72E+06 1.811 -4.20
 HOr+C4H9N_Olef=H2O+C4H8Nr_Olef_5
 5.72E+06 1.811 -4.20

!! Reaction Family: h abstractions OH* + H-C(H) (-CH3) (-CH2) - Sivaramakrishnan and Michael 2009

HOr+C4H8_Olef=H2O+C4H7r_Olef_4
 5.72E+06 1.811 -4.20
 HOr+CH3CH2CN=H2O+C3H4Nr_1
 5.72E+06 1.811 -4.20
 HOr+C2H5N_Olef=H2O+C2H4Nr_Olef
 5.72E+06 1.811 -4.20
 HOr+C2H5N_Olef=H2O+C2H4Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C3H5N_Olef=H2O+C3H4Nr_Olef
 5.72E+06 1.811 -4.20

HOr+C3H5N_Olef=H2O+C3H4Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C3H5N_Olef=H2O+C3H4Nr_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C3H6_Olef=H2O+C3H5r_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C3H6_Olef=H2O+C3H5r_Olef_3
 5.72E+06 1.811 -4.20
 HOr+C3H7N_2=H2O+C3H6Nr_4
 5.72E+06 1.811 -4.20
 HOr+C3H7N_Olef=H2O+C3H6Nr_Olef
 5.72E+06 1.811 -4.20
 HOr+C3H7N_Olef=H2O+C3H6Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C4H5N_Olef=H2O+C4H4Nr_Olef
 5.72E+06 1.811 -4.20
 HOr+C4H5N_Olef=H2O+C4H4Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_3
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_3
 5.72E+06 1.811 -4.20
 HOr+C4H8_Olef=H2O+C4H7r_Olef_1
 5.72E+06 1.811 -4.20
 HOr+C4H8_Olef=H2O+C4H7r_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C4H8_Olef_3=H2O+C4H7r_Olef_7
 5.72E+06 1.811 -4.20
 HOr+C4H9N_Olef=H2O+C4H8Nr_Olef_2
 5.72E+06 1.811 -4.20
 HOr+C4H9N_Olef=H2O+C4H8Nr_Olef_3
 5.72E+06 1.811 -4.20
 HOr+CH2CHCN=H2O+C3H2Nr_Olef_1
 5.72E+06 1.811 -4.20
 HOr+CH2CHCN=H2O+C3H2Nr_Olef_2
 5.72E+06 1.811 -4.20

!! Reaction Family: h abstractions OH* + H-C=R - Cai et al

HOr+C2H5N=H2O+C2H4Nr_3
 3.58E+10 0.76 -1.40
 HOr+C2H5N_1=H2O+C2H4Nr_3
 3.58E+10 0.76 -1.40
 HOr+C3H5N_Olef=H2O+C3H4Nr_Olef_3
 3.58E+10 0.76 -1.40
 HOr+C3H6_Olef=H2O+C3H5r_Olef_1
 3.58E+10 0.76 -1.40

HOr+C3H7N=H2O+C3H6Nr_2
 3.58E+10 0.76 -1.40
 HOr+C3H7N_1=H2O+C3H6Nr_2
 3.58E+10 0.76 -1.40
 HOr+C3H7N_Olef=H2O+C3H6Nr_Olef_3
 3.58E+10 0.76 -1.40
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_5
 3.58E+10 0.76 -1.40
 HOr+C4H7N_Olef=H2O+C4H6Nr_Olef_6
 3.58E+10 0.76 -1.40
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_5
 3.58E+10 0.76 -1.40
 HOr+C4H7N_Olef_1=H2O+C4H6Nr_Olef_6
 3.58E+10 0.76 -1.40
 HOr+C4H8_Olef=H2O+C4H7r_Olef_3
 3.58E+10 0.76 -1.40
 HOr+C4H8_Olef_1=H2O+C4H7r_Olef_5
 3.58E+10 0.76 -1.40
 HOr+C4H8_Olef_1=H2O+C4H7r_Olef_6
 3.58E+10 0.76 -1.40
 HOr+C4H8_Olef_2=H2O+C4H7r_Olef_5
 3.58E+10 0.76 -1.40
 HOr+C4H8_Olef_2=H2O+C4H7r_Olef_6
 3.58E+10 0.76 -1.40
 HOr+C4H9N=H2O+C4H8Nr_3
 3.58E+10 0.76 -1.40
 HOr+C4H9N_1=H2O+C4H8Nr_3
 3.58E+10 0.76 -1.40
 HOr+C4H9N_Olef=H2O+C4H8Nr_Olef_4
 3.58E+10 0.76 -1.40
 HOr+CH2CHCN=H2O+C3H2Nr_Olef
 3.58E+10 0.76 -1.40

!! Reaction Family: h abstractions HO2* + H-C(-N) - Sivaramakrishnan and Michael 2009

HO2r+C2H5N_2=H2O2+C2H4Nr_1
 1.260E2 3.37 57.4
 HO2r+C3H7N=H2O2+CH3CHNCH2
 1.260E2 3.37 57.4
 HO2r+C3H7N_1=H2O2+CH3CHNCH2
 1.260E2 3.37 57.4
 HO2r+C3H7N_2=H2O2+CH3CHNCH2
 1.260E2 3.37 57.4
 HO2r+C3H7N_Olef=H2O2+C3H6Nr_Olef_2
 1.260E2 3.37 57.4
 HO2r+C4H9N=H2O2+C4H8Nr
 1.260E2 3.37 57.4
 HO2r+C4H9N_1=H2O2+C4H8Nr
 1.260E2 3.37 57.4
 HO2r+C4H9N_Olef=H2O2+C4H8Nr_Olef
 1.260E2 3.37 57.4
 HO2r+CH5N=H2O2+CH4Nr
 1.260E2 3.37 57.4

!! Reaction Family: h abstractions HO2* + CH3 - Cai et al. (2016)

HO2r+C2H5N=H2O2+C2H4Nr_2
 6.63E+00 3.59 71.80

HO2r+C2H5N_1=H2O2+C2H4Nr_2
6.63E+00 3.59 71.80
HO2r+C3H6_Olef=H2O2+C3H5r_Olef
6.63E+00 3.59 71.80
HO2r+C3H7N=H2O2+C3H6Nr_1
6.63E+00 3.59 71.80
HO2r+C3H7N_1=H2O2+C3H6Nr_1
6.63E+00 3.59 71.80
HO2r+C3H7N_2=H2O2+C3H6Nr_3
6.63E+00 3.59 71.80
HO2r+CH3CH2CN=H2O2+C3H4Nr
6.63E+00 3.59 71.80
HO2r+CH3CN=H2O2+C2H2Nr
6.63E+00 3.59 71.80

!! Reaction Family: h abstractions HO2* + H-N - Lucassen et al.

HO2r+C2H5N=H2O2+C2H4Nr_4
2.80E+12 0.00 56.90
HO2r+C2H5N_1=H2O2+C2H4Nr_4
2.80E+12 0.00 56.90
HO2r+C2H5N_Olef=H2O2+C2H4Nr_2
1.53E3 2.85 24.61
HO2r+C3H7N_Olef=H2O2+C3H6Nr_1
1.53E3 2.85 24.61
HO2r+C4H9N_Olef=H2O2+C4H8Nr_Olef_5
1.53E3 2.85 24.61
HO2r+CH3N=H2O2+CH2Nr
2.80E+12 0.00 56.90
HO2r+CH5N=H2O2+CH4Nr_1
1.53E3 2.85 24.61

!! Reaction Family: h abstractions HO2* + CH2 - Cai et al. (2016)

HO2r+C4H8_Olef=H2O2+C4H7r_Olef_4
1.26E+02 3.37 57.40
HO2r+CH3CH2CN=H2O2+C3H4Nr_1
1.26E+02 3.37 57.40

!! Reaction Family: h abstractions HO2* + C=R - Cai et al. not optimized (2016)

HO2r+C2H5N=H2O2+C2H4Nr_3
2.80E+12 0.00 56.90
HO2r+C2H5N_1=H2O2+C2H4Nr_3
2.80E+12 0.00 56.90
HO2r+C2H5N_Olef=H2O2+C2H4Nr_Olef_2
2.80E+12 0.00 56.90
HO2r+C3H5N_Olef=H2O2+C3H4Nr_Olef_3
2.80E+12 0.00 56.90
HO2r+C3H6_Olef=H2O2+C3H5r_Olef_1
2.80E+12 0.00 56.90
HO2r+C3H7N=H2O2+C3H6Nr_2
2.80E+12 0.00 56.90
HO2r+C3H7N_1=H2O2+C3H6Nr_2
2.80E+12 0.00 56.90
HO2r+C3H7N_Olef=H2O2+C3H6Nr_Olef_3
2.80E+12 0.00 56.90
HO2r+C4H7N_Olef=H2O2+C4H6Nr_Olef_5
2.80E+12 0.00 56.90

HO2r+C4H7N_Olef=H2O2+C4H6Nr_Olef_6
 2.80E+12 0.00 56.90
 HO2r+C4H7N_Olef_1=H2O2+C4H6Nr_Olef_5
 2.80E+12 0.00 56.90
 HO2r+C4H7N_Olef_1=H2O2+C4H6Nr_Olef_6
 2.80E+12 0.00 56.90
 HO2r+C4H8_Olef=H2O2+C4H7r_Olef_3
 2.80E+12 0.00 56.90
 HO2r+C4H8_Olef_1=H2O2+C4H7r_Olef_5
 2.80E+12 0.00 56.90
 HO2r+C4H8_Olef_1=H2O2+C4H7r_Olef_6
 2.80E+12 0.00 56.90
 HO2r+C4H8_Olef_2=H2O2+C4H7r_Olef_5
 2.80E+12 0.00 56.90
 HO2r+C4H8_Olef_2=H2O2+C4H7r_Olef_6
 2.80E+12 0.00 56.90
 HO2r+C4H9N=H2O2+C4H8Nr_3
 2.80E+12 0.00 56.90
 HO2r+C4H9N_1=H2O2+C4H8Nr_3
 2.80E+12 0.00 56.90
 HO2r+C4H9N_Olef=H2O2+C4H8Nr_Olef_4
 2.80E+12 0.00 56.90
 HO2r+CH2CHCN=H2O2+C3H2Nr_Olef
 2.80E+12 0.00 56.90

!! Reaction Family: h abstractions O* + CH3 - Cai et al. (2016)

Or+C3H7N=HOR+CH3CHNCH2
 1.10E+06 2.45 11.8
 Or+C3H7N_1=HOR+CH3CHNCH2
 1.10E+06 2.45 11.8
 Or+C3H7N_2=HOR+CH3CHNCH2
 1.10E+06 2.45 11.8
 Or+C3H7N_Olef=HOR+C3H6Nr_Olef_2
 1.10E+06 2.45 11.8
 Or+C4H9N=HOR+C4H8Nr
 1.10E+06 2.45 11.8
 Or+C4H9N_1=HOR+C4H8Nr
 1.10E+06 2.45 11.8
 Or+C4H9N_Olef=HOR+C4H8Nr_Olef
 1.10E+06 2.45 11.8
 Or+CCNCC=HOR+CCjNCC
 1.10E+06 2.45 11.8
 Or+C2H5N=HOR+C2H4Nr_2
 1.10E+06 2.45 11.8
 Or+C2H5N_1=HOR+C2H4Nr_2
 1.10E+06 2.45 11.8
 Or+C3H6_Olef=HOR+C3H5r_Olef
 1.10E+06 2.45 11.8
 Or+C3H7N=HOR+C3H6Nr_1
 1.10E+06 2.45 11.8
 Or+C3H7N_1=HOR+C3H6Nr_1
 1.10E+06 2.45 11.8
 Or+C3H7N_2=HOR+C3H6Nr_3
 1.10E+06 2.45 11.8
 Or+C4H5N_Olef=HOR+C4H4Nr_Olef_2
 1.10E+06 2.45 11.8

Or+C4H7N_Olef=HOr+C4H6Nr_Olef_4
 1.10E+06 2.45 11.8
 Or+C4H7N_Olef_1=HOr+C4H6Nr_Olef_4
 1.10E+06 2.45 11.8
 Or+C4H8_Olef=HOr+C4H7r_Olef
 1.10E+06 2.45 11.8
 Or+C4H8_Olef_1=HOr+C4H7r_Olef_4
 1.10E+06 2.45 11.8
 Or+C4H8_Olef_2=HOr+C4H7r_Olef_4
 1.10E+06 2.45 11.8
 Or+C4H8_Olef_3=HOr+C4H7r_Olef_8
 1.10E+06 2.45 11.8
 Or+C4H9N=HOr+C4H8Nr_1
 1.10E+06 2.45 11.8
 Or+C4H9N=HOr+C4H8Nr_2
 1.10E+06 2.45 11.8
 Or+C4H9N=HOr+C4H8Nr_Olef_5
 1.10E+06 2.45 11.8
 Or+C4H9N_1=HOr+C4H8Nr_1
 1.10E+06 2.45 11.8
 Or+C4H9N_1=HOr+C4H8Nr_2
 1.10E+06 2.45 11.8
 Or+C4H9N_1=HOr+C4H8Nr_Olef_5
 1.10E+06 2.45 11.8
 Or+C4H9N_Olef=HOr+C4H8Nr_Olef_1
 1.10E+06 2.45 11.8
 Or+CCNCC=HOr+CjCNCC
 1.10E+06 2.45 11.8
 Or+CH3CH2CN=HOr+C3H4Nr
 1.10E+06 2.45 11.8
 Or+C3H7N_Olef=HOr+C3H6Nr_1
 1.10E+06 2.45 11.8
 Or+C4H9N_Olef=HOr+C4H8Nr_Olef_5
 1.10E+06 2.45 11.8
 Or+CCNCC=HOr+CCNjCC
 1.10E+06 2.45 11.8

!! Reaction Family: h abstractions O* + CH2 - Cai et al. (2016)

Or+C4H8_Olef=HOr+C4H7r_Olef_4
 1.19E+06 2.44 11.90
 Or+CH3CH2CN=HOr+C3H4Nr_1
 1.19E+06 2.44 11.90

!! Reaction Family: h abstractions O* + C=R - Cai et al. not optimized (2016)

Or+C2H5N=HOr+C2H4Nr_3
 5.000E+12 0.000 7.5
 Or+C2H5N_1=HOr+C2H4Nr_3
 5.000E+12 0.000 7.5
 Or+C2H5N_Olef=HOr+C2H4Nr_Olef_2
 5.000E+12 0.000 7.5
 Or+C3H5N_Olef=HOr+C3H4Nr_Olef_3
 5.000E+12 0.000 7.5
 Or+C3H6_Olef=HOr+C3H5r_Olef_1
 5.000E+12 0.000 7.5
 Or+C3H7N=HOr+C3H6Nr_2
 5.000E+12 0.000 7.5

Or+C3H7N_1=HOr+C3H6Nr_2
 5.000E+12 0.000 7.5
 Or+C3H7N_Olef=HOr+C3H6Nr_Olef_3
 5.000E+12 0.000 7.5
 Or+C4H7N_Olef=HOr+C4H6Nr_Olef_5
 5.000E+12 0.000 7.5
 Or+C4H7N_Olef=HOr+C4H6Nr_Olef_6
 5.000E+12 0.000 7.5
 Or+C4H7N_Olef_1=HOr+C4H6Nr_Olef_5
 5.000E+12 0.000 7.5
 Or+C4H7N_Olef_1=HOr+C4H6Nr_Olef_6
 5.000E+12 0.000 7.5
 Or+C4H8_Olef=HOr+C4H7r_Olef_3
 5.000E+12 0.000 7.5
 Or+C4H8_Olef_1=HOr+C4H7r_Olef_5
 5.000E+12 0.000 7.5
 Or+C4H8_Olef_1=HOr+C4H7r_Olef_6
 5.000E+12 0.000 7.5
 Or+C4H8_Olef_2=HOr+C4H7r_Olef_5
 5.000E+12 0.000 7.5
 Or+C4H8_Olef_2=HOr+C4H7r_Olef_6
 5.000E+12 0.000 7.50
 Or+C4H9N=HOr+C4H8Nr_3
 5.000E+12 0.000 7.50
 Or+C4H9N_1=HOr+C4H8Nr_3
 5.000E+12 0.000 7.50
 Or+C4H9N_Olef=HOr+C4H8Nr_Olef_4
 5.000E+12 0.000 7.50
 Or+CH2CHCN=HOr+C3H2Nr_Olef
 5.000E+12 0.000 7.50

!! Reaction Family: h abstractions O2** + CH3 - Cai 2016

O2+C2H5N=HO2r+C2H4Nr_2
 5.94E+12 0.00 218.80
 O2+C2H5N_1=HO2r+C2H4Nr_2
 5.94E+12 0.00 218.80
 O2+C2H5N_2=HO2r+C2H4Nr_1
 5.94E+12 0.00 218.80
 O2+C3H6_Olef=HO2r+C3H5r_Olef
 5.94E+12 0.00 218.80
 O2+C3H7N=HO2r+C3H6Nr_1
 5.94E+12 0.00 218.80
 O2+C3H7N=HO2r+CH3CHNCH2
 5.94E+12 0.00 218.80
 O2+C3H7N_1=HO2r+C3H6Nr_1
 5.94E+12 0.00 218.80
 O2+C3H7N_1=HO2r+CH3CHNCH2
 5.94E+12 0.00 218.80
 O2+C3H7N_2=HO2r+C3H6Nr_3
 5.94E+12 0.00 218.80
 O2+C3H7N_Olef=HO2r+C3H6Nr_Olef_2
 5.94E+12 0.00 218.80
 O2+C4H5N_Olef=HO2r+C4H4Nr_Olef_2
 5.94E+12 0.00 218.80
 O2+C4H7N_Olef=HO2r+C4H6Nr_Olef_4
 5.94E+12 0.00 218.80
 O2+C4H7N_Olef_1=HO2r+C4H6Nr_Olef_4
 5.94E+12 0.00 218.80

O2+C4H8_Olef=HO2r+C4H7r_Olef
5.94E+12 0.00 218.80
O2+C4H8_Olef_1=HO2r+C4H7r_Olef_4
5.94E+12 0.00 218.80
O2+C4H8_Olef_2=HO2r+C4H7r_Olef_4
5.94E+12 0.00 218.80
O2+C4H8_Olef_3=HO2r+C4H7r_Olef_8
5.94E+12 0.00 218.80
O2+C4H9N=HO2r+C4H8Nr_1
5.94E+12 0.00 218.80
O2+C4H9N=HO2r+C4H8Nr_2
5.94E+12 0.00 218.80
O2+C4H9N=HO2r+C4H8Nr_Olef_5
5.94E+12 0.00 218.80
O2+C4H9N_1=HO2r+C4H8Nr_1
5.94E+12 0.00 218.80
O2+C4H9N_1=HO2r+C4H8Nr_2
5.94E+12 0.00 218.80
O2+C4H9N_1=HO2r+C4H8Nr_Olef_5
5.94E+12 0.00 218.80
O2+C4H9N_Olef=HO2r+C4H8Nr_Olef_1
5.94E+12 0.00 218.80
O2+CCNCC=HO2r+CjCNCC
5.94E+12 0.00 218.80
O2+CH3CH2CN=HO2r+C3H4Nr
5.94E+12 0.00 218.80
O2+CH3CN=HO2r+C2H2Nr
5.94E+12 0.00 218.80
O2+CH5N=HO2r+CH4Nr
5.94E+12 0.00 218.80

!! Reaction Family: h abstractions O2** + CH2 - Cai 2016

O2+C3H7N_2=HO2r+CH3CHNCH2
1.34E+13 0.00 207.70
O2+C4H8_Olef=HO2r+C4H7r_Olef_4
1.34E+13 0.00 207.70
O2+C4H9N=HO2r+C4H8Nr
1.34E+13 0.00 207.70
O2+C4H9N_1=HO2r+C4H8Nr
1.34E+13 0.00 207.70
O2+C4H9N_Olef=HO2r+C4H8Nr_Olef
1.34E+13 0.00 207.70
O2+CCNCC=HO2r+CCjNCC
1.34E+13 0.00 207.70
O2+CH3CH2CN=HO2r+C3H4Nr_1
1.34E+13 0.00 207.70
O2+CCNCC=HO2r+CCNjCC
1.34E+13 0.00 207.70

!! Reaction Family: Carbon-Centered Beta-Scission (non-cyclic molecules) onto a carbon-centered radical

C3H7r=C2H4_Olef+CH3r
7.05E+13 0.00 129.00
C4H7r_Olef=C2H3r_Olef+C2H4_Olef
6.93E+13 0.00 153.00
C4H9r=C2H4_Olef+C2H5r
5.06E+13 0.00 120.00

C4H9r_1=C3H6_Olef+CH3r	1.11E+14	0.00	129.00	
C4H9r_2=C3H6_Olef+CH3r	1.57E+14	0.00	129.00	
C2H5N_Olef+Hr=C2H6Nr_3	7.26E+13	0.00	23.90	
C3H5N_Olef+Hr=C3H6Nr_3	7.26E+13	0.00	23.90	
C3H5N_Olef+Hr=CH3CHNCH2	5.03E+13	0.00	11.50	
C3H6_Olef+Hr=C3H7r	1.17E+08	1.68	8.490	
C3H7r_1=C3H6_Olef+Hr	0.493	165.73		8.45E+12
C3H7N_Olef+Hr=C3H8Nr	5.56E+13	0.00	16.10	
C3H7N_Olef+Hr=C3H8Nr_1	7.26E+13	0.00	23.90	
C4H5N_Olef+Hr=C4H6Nr_1	2.29E+13	0.00	30.90	
C4H5N_Olef+Hr=C4H6Nr_2	2.29E+13	0.00	30.90	
C4H5N_Olef+Hr=C4H6Nr_3	5.60E+13	0.00	11.60	
C4H7N_Olef+Hr=C4H8Nr	5.03E+13	0.00	11.50	
C4H7N_Olef+Hr=C4H8Nr_1	7.26E+13	0.00	23.90	
C4H7N_Olef+Hr=C4H8Nr_2	7.26E+13	0.00	23.90	
C4H7N_Olef_1+Hr=C4H8Nr	5.03E+13	0.00	11.50	
C4H7N_Olef_1+Hr=C4H8Nr_1	7.26E+13	0.00	23.90	
C4H7N_Olef_1+Hr=C4H8Nr_2	7.26E+13	0.00	23.90	
C4H8_Olef+Hr=C4H9r	6.46E+13	0.00	22.50	
C4H8_Olef+Hr=C4H9r_1	5.56E+13	0.00	16.10	
C4H8_Olef_1+Hr=C4H9r_1	1.35E+14	0.00	20.10	
C4H8_Olef_2+Hr=C4H9r_1	1.35E+14	0.00	20.10	
C4H8_Olef_3+Hr=C4H9r_2	3.66E+13	0.00	25.90	
C4H8_Olef_3+Hr=C4H9r_3	1.28E+14	0.00	13.60	
C4H9N_Olef+Hr=CCjNCC	5.56E+13	0.00	16.10	
C4H9N_Olef+Hr=CjCNCC	7.26E+13	0.00	23.90	
CH2CHCN+Hr=C3H4Nr	7.35E+13	0.00	26.10	
CH2CHCN+Hr=C3H4Nr_1	4.99E+13	0.00	13.10	

!! Reaction Family: h abstractions H* + H-N

Hr+C2H5N=H2+C2H4Nr_4
 7.37E+13 0.00 25.10
 Hr+C2H5N_1=H2+C2H4Nr_4
 7.37E+13 0.00 25.10
 Hr+C3H7N_Olef=H2+C3H6Nr_1
 1.25E+14 0.00 42.10
 Hr+C4H9N_Olef=H2+C4H8Nr_Olef_5
 1.25E+14 0.00 42.10
 Hr+CCNCC=H2+CCNjCC
 1.74E+12 0.00 19.76
 C3H6Nr_3=C2H4_Olef+CH2Nr
 2.12E+10 0.85 89.20
 C3H8Nr_1=C2H4_Olef+CH4Nr_1
 2.12E+10 0.85 89.20
 C4H8Nr_1=C2H4_Olef+C2H4Nr_4
 2.12E+10 0.85 89.20
 C4H8Nr_2=C2H4_Olef+C2H4Nr_4
 2.12E+10 0.85 89.20
 C4H8Nr_Olef_1=C2H4Nr_2+C2H4_Olef
 2.12E+10 0.85 89.20
 CjCNCC=C2H4_Olef+C2H6Nr
 2.12E+10 0.85 89.20
 C3H6Nr_Olef_2=C2H3r_Olef+CH3N
 1.46E+14 -0.01 117.00
 C3H8Nr=C2H5N+CH3r
 7.31E+13 -0.01 117.00
 C3H8Nr=C2H5N_1+CH3r
 7.31E+13 -0.01 117.00
 C3H8Nr_2=C2H5r+CH3N
 1.46E+14 -0.01 117.00
 C4H8Nr_Olef=C2H3r_Olef+C2H5N
 7.31E+13 -0.01 117.00
 C4H8Nr_Olef=C2H3r_Olef+C2H5N_1
 7.31E+13 -0.01 117.00
 CCjNCC=C2H5N+C2H5r
 7.31E+13 -0.01 117.00
 CCjNCC=C2H5N_1+C2H5r
 7.31E+13 -0.01 117.00
 C2H6Nr_2=C2H5N+Hr
 1.13E+10 0.99 137.80
 C2H6Nr_2=C2H5N_1+Hr
 1.13E+10 0.99 137.80
 C3H6Nr=CH3CH2CN+Hr
 1.13E+10 0.99 137.80
 C3H6Nr_Olef_2=C3H5N_Olef+Hr
 2.26E+10 0.99 137.80
 C3H8Nr=C3H7N+Hr
 1.13E+10 0.99 137.80
 C3H8Nr=C3H7N_1+Hr
 1.13E+10 0.99 137.80
 C3H8Nr_2=C3H7N_2+Hr
 1.00E+10 0.99 137.80
 C4H8Nr_Olef=C4H7N_Olef+Hr
 1.13E+10 0.99 137.80
 C4H8Nr_Olef=C4H7N_Olef_1+Hr
 1.13E+10 0.99 137.80
 CCjNCC=C4H9N+Hr
 1.13E+10 0.99 137.80

CCjNCC=C4H9N_1+Hr
1.13E+10 0.99 137.80

!! Reaction Family: C-H beta scission of a nitrogen-centered radical
N*-C-H

C2H6Nr=C2H5N+Hr
4.53E+09 1.33 138.90

C2H6Nr=C2H5N_1+Hr
4.53E+09 1.33 138.90

C4H8Nr_Olef_5=C4H7N_Olef+Hr
4.53E+09 1.33 138.90

C4H8Nr_Olef_5=C4H7N_Olef_1+Hr
4.53E+09 1.33 138.90

CCNjCC=C4H9N+Hr
6.04E+09 1.33 138.90

CCNjCC=C4H9N_1+Hr
6.04E+09 1.33 138.90

!! Reaction Family: C-H beta scission of a nitrogen-centered radical -
N=C-H

C2H4Nr_4=CH3CN+Hr
1.43E+14 0.00 124.60

C4H8Nr_Olef_5=C3H5N_Olef+CH3r
1.47E+10 1.19 113.30

CCNjCC=CH3r+C3H7N_2
1.96E+10 1.19 113.30

!! Reaction Family: C-C scission reaction

CH3r+C3H8Nr=CCNCC
1.00E+13 0.00 0.00

!! Reaction Family: C-H scission reaction

CCjNCC+Hr=CCNCC
2.00E+13 0.00 0.00

!! Reaction Family: C-N scission reaction

C2H5r+C2H6Nr=CCNCC
1.0E+13 0.00 0.00

!! Reaction Family: Unimolecular elimination reaction

CCNCC=C2H4_Olef+C2H7N
2.00E+11 0.00 281.90

!! Reaction Family: CCC#N formation reaction

c-C3H5N+Hr=CH3CHNCH2
9.80E+09 0.00 0.00

CH3CHCN(S)=c-C3H5N
3.00E+13 0.00 16.70

CH3CHCN(S)=CH3CH2CN
3.00E+13 0.00 33.50

c-C3H5N=CH3CH2CN
4.70E+13 0.00 173.60

!! Reaction Family: CC#N formation reaction

c-C2H3N+Hr=C2H4Nr_4
9.80E+09 1.21 8.20

c-C2H3N+Hr=C2H4Nr
1.10E+10 1.23 10.10

$C2H4Nr=C2H4Nr_4$
 1.30E+45 -10.07 276.60
 $CH2CHN(S)=c-C2H3N$
 3.00E+13 0.00 16.70
 $CH2CHN(S)=CH3CN$
 3.00E+13 0.00 33.50
 $CH3r+CH3N=CH4+CHNHr$
 1.36E+13 0.00 61.40
 $HOr+H3N=H2O+H2Nr$
 7.20E+06 2.00 1.90
 $CH3r+C2H5N_Olef=CH4+C2H4Nr_Olef_2$
 1.10E+13 0.00 78.50
 $HOr+CH5N=H2O+CH4Nr$
 4.20E+13 0.00 0.00

!! CH3 recombination
 $CH3r+CH3r=C2H6$
 2.00E+13 0.00 0.00
 $C2H5r+CH3r=C3H8$
 2.00E+13 0.00 0.00
 $HO2r+C2H6=H2O2+C2H5r$
 6.63E+00 3.59 71.80
 $CH3r+CH5N=CH4+CH4Nr_1$
 3.71E+12 0.00 60.80
 $HOr+C2H5N_Olef=H2O+C2H4Nr_2$
 2.40E+06 2.00 1.90
 $Hr+C2H5N_Olef=H2+C2H4Nr_2$
 3.16E+13 0.00 46.90
 $H2Nr+CH3N=H3N+CH2Nr$
 7.82E+12 0.00 27.70

!! Reaction Family: N-C beta scission of a carbon-centered radical -
 C^*-N-C
 $C2H6Nr_1=CH3N+CH3r$
 1.46E+14 -0.01 117.00
 $CH3r+C2H5N_2=CH4+C2H4Nr_1$
 2.84E+13 0.00 60.60

!! Reaction Family: C-C beta scission of a nitrogen-centered radical -
 N^*-C-C
 $C2H6Nr=CH3r+CH3N$
 1.47E+10 1.19 113.30
 $CH3r+CH5N=CH4+CH4Nr$
 2.79E+13 0.00 63.50
 $Hr+C2H5N_2=H2+C2H4Nr$
 1.42E+14 0.00 42.70
 $CHNHr=HCN+Hr$
 1.79E+14 0.00 118.90

!! Reaction Family: Intramolecular h abstractions to a carbon centered
 group by a carbon radical
 $C2H4Nr_1=C2H4Nr$
 1.30E+45 -10.07 276.60
 $Or+CH5N=HOr+CH4Nr_1$
 3.30E+08 1.50 26.60

!! Reaction Family: Hydrogen Radical Addition (non-cyclic components)
 by MK Sabbe (Hydrogen Radical Additions to Unsaturated Hydrocarbons and

the Reverse beta-Scission Reactions: Modeling of Activation Energies and Pre-Exponential Factors. ChemPhysChem 11 (2010) 195)

C2H5r=C2H4_olef+Hr
1.5E+9 1.55 150.62

CH3r+C2H5N_2=CH4+C2H4Nr
1.36E+13 0.00 61.40

HOr+CH3N=H2O+CHNHr
2.86E+06 1.81 -4.20

Or+C2H6=HOr+C2H5r
2.09E+06 2.42 19.90

CH4Nr=CH3N+Hr
2.26E+10 0.99 137.80

Hr+CH4=H2+CH3r
4.82E+14 0.00 66.40

!! Reaction Family: h abstractions OH* + H-C(H) (-CH2) (-CH2) - Sivaramakrishnan and Michael 2009

!!HOr+C2H4_olef=H2O+C2H3r_olef
1.14E+07 1.81 -4.20

HOr+C2H4_olef=H2O+C2H3r_olef
2.230E+04 2.745 9.27

Hr+CH3N=H2+CH2Nr
7.37E+13 0.00 25.10

HOr+CH5N=H2O+CH4Nr_1
2.40E+06 2.00 1.90

Hr+H3N=H2+H2Nr
1.90E+14 0.00 65.40

HOr+CH3CN=H2O+C2H2Nr
1.36E+07 1.81 3.10

!! Reaction Family: h abstractions O* + H-N - Lucassen et al.

Or+C2H5N_olef=HOr+C2H4Nr_2
3.30E+08 1.50 26.60

O2+C2H6=HO2r+C2H5r
5.94E+12 0.00 218.80

c-C2H3N=CH3CN
4.70E+13 0.00 173.60

Or+CH5N=HOr+CH4Nr
6.80E+12 0.00 5.30

H2Nr+C2H5N_olef=H3N+C2H4Nr_2
2.95E+12 0.00 33.10

Hr+CH3N=H2+CHNHr
1.42E+14 0.00 42.70

Or+H3N=HOr+H2Nr
3.30E+08 1.50 26.60

HOr+CH3N=H2O+CH2Nr
2.40E+06 2.00 1.90

HOr+C2H5N_olef=H2O+C2H4Nr_olef_2
3.58E+10 0.76 -1.40

!! Reaction Family: h abstractions O* + H-C(-N) - Lucassen et al.

Or+C2H5N_2=HOr+C2H4Nr_1
6.80E+12 0.00 5.30

C2H5N_olef+Hr=C2H6Nr_2
5.56E+13 0.00 16.10

Hr+C2H5N_2=H2+C2H4Nr_1
1.46E+14 0.00 45.60

$\text{CH}_3\text{r} + \text{CH}_3\text{CN} = \text{CH}_4 + \text{C}_2\text{H}_2\text{Nr}$
 2.38E+13 0.00 60.90
 $\text{C}_2\text{H}_6\text{Nr}_1 = \text{C}_2\text{H}_5\text{N}_2 + \text{Hr}$
 2.26E+10 0.99 137.80
 $\text{Hr} + \text{CH}_5\text{N} = \text{H}_2 + \text{CH}_4\text{Nr}_1$
 3.39E+13 0.00 48.40
 $\text{CH}_2\text{Nr} = \text{HCN} + \text{Hr}$
 4.12E+14 0.00 138.70
 $\text{Or} + \text{CH}_3\text{CN} = \text{HOr} + \text{C}_2\text{H}_2\text{Nr}$
 2.09E+06 2.42 19.90
 $\text{HO}_2\text{r} + \text{H}_3\text{N} = \text{H}_2\text{O}_2 + \text{H}_2\text{Nr}$
 2.86E+00 1.81 -4.20
 $\text{HOr} + \text{C}_2\text{H}_6 = \text{H}_2\text{O} + \text{C}_2\text{H}_5\text{r}$
 2.73E+07 1.81 3.10
 $\text{HOr} + \text{C}_2\text{H}_5\text{N}_2 = \text{H}_2\text{O} + \text{C}_2\text{H}_4\text{Nr}$
 2.86E+06 1.81 -4.20
 $\text{CH}_3\text{r} + \text{C}_2\text{H}_5\text{N}_\text{Olef} = \text{CH}_4 + \text{C}_2\text{H}_4\text{Nr}_2$
 1.84E+12 0.00 57.80
 $\text{CH}_4\text{Nr}_1 = \text{CH}_3\text{N} + \text{Hr}$
 1.56E+14 0.00 145.10
 $\text{Hr} + \text{C}_2\text{H}_5\text{N}_\text{Olef} = \text{H}_2 + \text{C}_2\text{H}_4\text{Nr}_\text{Olef}_2$
 5.03E+13 0.00 65.90

!! Reaction Family: h abstractions $\text{OH}^* + \text{H-C(-N)}$ - Lucassen et al.
 $\text{HOr} + \text{C}_2\text{H}_5\text{N}_2 = \text{H}_2\text{O} + \text{C}_2\text{H}_4\text{Nr}_1$
 4.20E+13 0.00 0.00

!! Reaction Family: h abstractions $\text{H}^* + \text{C-H}$
 $\text{Hr} + \text{C}_2\text{H}_4_\text{Olef} = \text{H}_2 + \text{C}_2\text{H}_3\text{r}_\text{Olef}$
 7.88E+14 0.00 72.10
 $\text{H}_2\text{Nr} + \text{CH}_5\text{N} = \text{H}_3\text{N} + \text{CH}_4\text{Nr}_1$
 2.95E+12 0.00 33.10
 $\text{Hr} + \text{CH}_5\text{N} = \text{H}_2 + \text{CH}_4\text{Nr}$
 1.56E+14 0.00 36.20

!! Reaction Family: N-H beta scission of a carbon-centered radical - $\text{C}^*-\text{N}-\text{H}$
 $\text{C}_2\text{H}_4\text{Nr}_3 = \text{CH}_3\text{CN} + \text{Hr}$
 1.22E+14 0.00 91.30
 $\text{CH}_3\text{r} + \text{H}_3\text{N} = \text{CH}_4 + \text{H}_2\text{Nr}$
 1.16E+13 0.00 75.50
 $\text{CH}_4\text{Nr} + \text{H}_3\text{N} = \text{CH}_5\text{N} + \text{H}_2\text{Nr}$
 1.02E+13 0.00 75.50

!! Reaction Family: C-N beta scission of a carbon-centered radical - $\text{C}^*-\text{C}-\text{N}$
 $\text{C}_2\text{H}_6\text{Nr}_3 = \text{C}_2\text{H}_4_\text{Olef} + \text{H}_2\text{Nr}$
 2.12E+10 0.85 89.20
 $\text{C}_2\text{H}_3\text{r}_\text{Olef} + \text{CH}_4 = \text{C}_2\text{H}_4_\text{Olef} + \text{CH}_3\text{r}$
 3.25E+13 0.00 64.40
 $\text{CHNHr} + \text{H}_3\text{N} = \text{CH}_3\text{N} + \text{H}_2\text{Nr}$
 5.24E+12 0.00 75.50
 $\text{C}_2\text{H}_5\text{r} + \text{H}_3\text{N} = \text{C}_2\text{H}_6 + \text{H}_2\text{Nr}$
 1.10E+13 0.00 75.50
 $\text{C}_2\text{H}_3\text{r}_\text{Olef} + \text{H}_3\text{N} = \text{C}_2\text{H}_4_\text{Olef} + \text{H}_2\text{Nr}$
 6.04E+12 0.00 75.50

!! additional recombinations

C2H5r+CN=CH3CH2CN
 1.0E+12 0.00 0.00 !
 CH3r+C2H2Nr=CH3CH2CN
 1.0E+12 0.00 0.00 !
 C2H3r_Olef+CN=CH2CHCN
 1.0E+12 0.00 0.00 !
 Hr+Hr=H2
 9.45E+13 -0.54 0.60
 C2H5r+Hr=C2H6
 2.00E+13 0.00 0.00
 C3H7r+Hr=C3H8
 2.00E+13 0.00 0.00

O2+CCjNCC=CCOjNCC
 1.04E+15 -0.92 -0.50
 !!Path 1: 1,3-shift + beta-scission
 CCOjNCC=CCdONCC+HOr
 1.14E-2 4.251 120.7

!!Path 2: 1,5-shift + beta-scission
 CCOjNCC=CCOONCjC
 0.25E-3 4.188 46.42

CCOONCjC=CH3CHO+HOr+C2H5N
 0.7E-01 3.67 27.96
 CCOONCjC=CH3CHO+HOr+C2H5N_1
 0.7E-01 3.67 27.96

!! Path 3: 1,4-shift + beta-scission
 CCOjNCC=CCOONjCC
 1.4E-2 4.232 96.44
 CCOONjCC=OOCdNCC+CH3r
 8.47E12 0.057 68.24

C3H6Nr_4+HO2r=OOCdNCC
 1.00E+13 0.000 0.00
 OdCdNCC+Hr=OjCdNCC
 1.00E+13 0.000 0.00
 HOr+CCdONCC=H2O+CCdONjCC
 1.360E+07 1.813 3.10
 HO2r+CCdONCC=H2O2+CCdONjCC
 1.53E+03 2.856 24.61
 O2+CCdONCC=HO2r+CCdONjCC
 2.56E+06 2.14 140.40
 CH3r+CCdONCC=CH4+CCdONjCC
 8.11E+11 0.00 29.80
 Hr+CCdONCC=H2+CCdONjCC
 1.74E+12 0.00 19.76
 CCdONjCC=CH3r+OdCdNCC
 1.96E+10 1.19 113.30

HO2r+CCNCC=H2O2+CjCNCC
 6.63E00 3.59 71.80
 HO2r+CCNCC=H2O2+CCjNCC
 1.08E+01 3.425 17.70

HO2r+CCNCC=H2O2+CCNjCC			
1.040E+02	3.196	20.90	
HOr+CCNCC=H2O+CCjNCC			
4.06E-01	4.224	-23.9	
HOr+CCNCC=H2O+CjCNCC			
6.09E-01	4.224	-23.9	
HOr+CCNCC=H2O+CCNjCC			
1.02E-01	4.224	-23.9	

END