

Appendix A

Reduced Chemical Scheme

Denomination for the organic peroxy operators

The different types of <peroxy> operators

<RO2> : successive NO/NO₂ conversions, final restitution of HO₂

<OHRO2> : successive NO/NO₂ conversions, final restitution of OH

<2NO2> : successive NO/NO₂ conversions, final restitution of NO₂

<NONO2> : successive NO/NO₂ conversions

<NONO2_C> : successive NO/NO₂ conversions, final restitution of CH₃O₂

<NITR> : NO removal and formation of a nitrate species

Information in the operator's names

↗ type of operator

<xRO2_ab...n>

↓

↘ type of <peroxy> that will be successively produced

number of NO/NO₂ conversions

ab..n are the following numbers or letters representing the type of <peroxy>:

2=alkylperoxy, peroxy permutation reactions considered;

7=alkylperoxy, no peroxy permutation reactions considered;

A=acylperoxy;

C=methylperoxy.

List of the species

Species invoked in the operators treatment

PAN2NONO2AC	surrogate species representing PAN (0C)
CA2NONO2AC	surrogate species representing the carboxylic acids (0C)
PA2NONO2AC	surrogate species representing the peracides (0C)
HP2RO2_22	surrogate species representing an hydroperoxyde (0C)
HP1NITR02	surrogate species representing an hydroperoxyde (0C)
OPEALC	surrogate species representing an alcohol (0C))
<1RO2_2>	operator giving HO ₂ after one NO/NO ₂ conversion
<1RO2_7>	operator giving HO ₂ after one NO/NO ₂ conversion
<1RO2_A>	operator giving HO ₂ after one NO/NO ₂ conversion
<2RO2_2A>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_A2>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_22>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_72>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_27>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_77>	operator giving HO ₂ after two NO/NO ₂ conversions
<2RO2_A7>	operator giving HO ₂ after two NO/NO ₂ conversions
<3RO2_727>	operator giving HO ₂ after three NO/NO ₂ conversions
<3RO2_772>	operator giving HO ₂ after three NO/NO ₂ conversions
<3RO2_722>	operator giving HO ₂ after three NO/NO ₂ conversions
<3RO2_2A2>	operator giving HO ₂ after three NO/NO ₂ conversions
<1_2NO2_2>	operator giving NO ₂ after one NO/NO ₂ conversion
<1_2NO2_7>	operator giving NO ₂ after one NO/NO ₂ conversion
<1_2NO2_A>	operator giving NO ₂ after one NO/NO ₂ conversion
<2_2NO2_2A>	operator giving NO ₂ after two NO/NO ₂ conversions
<2_2NO2_72>	operator giving NO ₂ after two NO/NO ₂ conversions
<1OHR02_2>	operator giving OH after one NO/NO ₂ conversion
<2OHR02_A2>	operator giving OH after two NO/NO ₂ conversions NO/NO ₂
<1NONO2_2>	operator converting NO to NO ₂
<1NONO2_7>	operator converting NO to NO ₂
<1NONO2_A>	operator converting NO to NO ₂
<2NONO2_7C>	operator converting NO to NO ₂
<2NONO2_2C>	operator converting NO to NO ₂
<2NONO2_AC>	operator converting NO to NO ₂
<3NONO2_2AC>	operator converting NO to NO ₂
<3NONO2_AAC>	operator converting NO to NO ₂
<1NITR01#2>	operator giving a surrogate nitrate
<1NITR01#7>	operator giving a surrogate nitrate
<1NITR02#2>	operator giving a surrogate nitrate
<1NITR02#7>	operator giving a surrogate nitrate
<1N03001#2>	operator giving a surrogate nitrate
<1N03001#7>	operator giving a surrogate nitrate
R2O2	operator R2O2 from Carter (SAPRC99)
RO2N	operator RO2N from Carter (SAPRC99)
RO2R	operator RO2R from Carter (SAPRC99)
NITR01	surrogate nitrate
NITR02	surrogate nitrate

Inorganic species

O3	O3
H2	H2
H2O2	H2O2
HNO2	HNO2

HNO4	HNO4
HO	HO
HO2	HO2
N2O5	N2O5
NO	NO
NO2	NO2
NO3	NO3
O1D	O1D
O3P	O3P
SO2	SO2
SULF	SULF
XC	lost carbon
CO	CO
CO2	CO2
HNO3	HNO ₃
XN2	lost nitrogen

Organic C1 species

CH4	CH4
HCOOH	HCO(OH)
CH2O	HCHO
CH3OH	CH3(OH)
CH3OOH	CH3(OOH)
CH3O2	CH3(OO.)

Species from the Carter's parameterization (SAPRC99)

T124B	124_trimethylbenzene
BUTYN	2_butyne
ACTYN	acetylene
APIN	alphapinene
DCB1	fragment from the DCB1 aromatic degradation
DCB2	fragment from the DCB2 aromatic degradation
DCB3	fragment from the DCB3 aromatic degradation
BALD	benzaldehyde
BENZ	benzene
BZCOO2	benzylacylperoxy
CRES	cresol
ETBNZ	ethylbenzene
LIMO	limonene
XN	lost nitrogen
NPHE	nitrophenol
BZNO2O	nitrophenoxy
PBZN	peroxybenzylnitrate
PHEN	phenol
BZO	phenoxy
TOL	toluene

Primary and secondary organic species

DO2000	CH2(OH)CHO
DK3000	CH2(OH)COCHO
ND2000	CH2(ONO2)CHO
NN3001	CH2(ONO2)COCH2(ONO2)
ND3000	CH2(ONO2)COCHO
NU4000	CH2(ONO2)COCH=CH2
NU3000	CH2(ONO2)CH=CH2
EK5001	CH3CH(CH3)-O-COCH3

C08005	CH ₃ CH(CH ₃)CH ₂ CH ₂ CH ₂ CH ₂ CH ₃
C06001	CH ₃ CH(CH ₃)CH ₂ CH ₂ CH ₃
K06001	CH ₃ CH(CH ₃)CH ₂ COCH ₃
C04001	CH ₃ CH(CH ₃)CH ₃
D04001	CH ₃ CH(CH ₃)CHO
N03001	CH ₃ CH(ONO ₂)CH ₃
N03002	CH ₃ CH(ONO ₂)CHO
O02000	CH ₃ CH ₂ (OH)
EK4000	CH ₃ CH ₂ -O-COCH ₃
H03000	CH ₃ CH ₂ CH ₂ (OOH)
N05001	CH ₃ CH ₂ CH ₂ CH(ONO ₂)CH ₃
EK6000	CH ₃ CH ₂ CH ₂ CH ₂ -O-COCH ₃
C08000	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃
C06000	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃
K06000	CH ₃ CH ₂ CH ₂ CH ₂ COCH ₃
C04000	CH ₃ CH ₂ CH ₂ CH ₃
D04000	CH ₃ CH ₂ CH ₂ CHO
C03000	CH ₃ CH ₂ CH ₃
D03000	CH ₃ CH ₂ CHO
A03000	CH ₃ CH ₂ CO(OH)
G03000	CH ₃ CH ₂ CO(OOH)
K04000	CH ₃ CH ₂ COCH ₃
U05004	CH ₃ CH ₂ C(CH ₃)=CH ₂
U04000	CH ₃ CH ₂ CH=CH ₂
C02000	CH ₃ CH ₃
D02000	CH ₃ CHO
A02000	CH ₃ CO(OH)
EK3000	CH ₃ CO-O-CH ₃
ED3000	CH ₃ CO-O-CHO
NK3000	CH ₃ COCH ₂ (ONO ₂)
HK3000	CH ₃ COCH ₂ (OOH)
ACETO	CH ₃ COCH ₃
MGLYO	CH ₃ COCHO
BIACE	CH ₃ COCOCH ₃
MVKET	CH ₃ COCH=CH ₂
U05003	CH ₃ C(CH ₃)=CHCH ₃
MEACR	CH ₃ C(CHO)=CH ₂
U04002	CH ₃ CH=CHCH ₃
GLYOX	CHOCHO
DD3002	CHOCOCHO
AN2000	CO(OH)CH ₂ (ONO ₂)
AD3000	CO(OH)CH ₂ CHO
AD2000	CO(OH)CHO
ISO	CH ₂ =C(CH ₃)CH=CH ₂
U02000	CH ₂ =CH ₂
U03000	CH ₂ =CHCH ₃
ACROL	CH ₂ =CHCHO

Counter species for peroxy permutation reactions

C_PERO2	= <1NITR03#2> + <1RO2_2> + <1N03001#2> + <2RO2_2A> + <2RO2_22> + <1NONO2_2> + <2RO2_27> + <1NITR01#2> + <1NITR02#2> <1_2NO2_2> + <3NONO2_2AC> + <3RO2_2A2> + <2NONO2_2C> + <1OHRO2_2> + <2_2NO2_2A> + R2O2 + RO2N + RO2R
C_PERO9	= <2NONO2_AC> + <2RO2_A2> + <1NONO2_A> + <2RO2_A7> + <3NONO2_AAC> + <1RO2_A> + <1_2NO2_A> + <2OHRO2_A2> + BZCOO2

HO_x/NO_x/O_x/CO reactions

Table A.1: *Reactions for inorganic species - Kinetic rates on the form $k=A.T^n.exp(-E_a/RT)$*

Bimolecular reactions	A (a)	n	E _a /R (b)	References and notes
O ³ P + O ₂ + M => O ₃	5.28E-28	-2.4	0.	Sander et al. [2000]
O ³ P + O ₃ => 2 O ₂	8.0E-12	0.	2060.	De More et al. [1997]
O ³ P + NO ₂ => NO	5.6E-12	0.	-180	Sander et al. [2000]
O ¹ D + H ₂ O => 2 HO	2.2E-10	0.	0.	Sander et al. [2000]
O ¹ D + M => O ³ P + M	2.09E-11	0.	-96	Carter [2000] (1)
O ₃ + NO => NO ₂	3.0E-12	0.	1500	Sander et al. [2000]
O ₃ + NO ₂ => NO ₃	1.2E-13	0.	2450	De More et al. [1997]
NO + NO ₃ => 2 NO ₂	1.5E-11	0.	-170	De More et al. [1997]
NO + NO + M => 2 NO ₂	3.30E-39	0.	-530	Atkinson et al. [1997]
NO ₂ + NO ₃ => NO + NO ₂	4.50E-14	0.	1260	De More et al. [1997]
HO + HNO ₂ => NO ₂	1.8E-11	0.	390	De More et al. [1997]
HO + NO ₃ => HO ₂ + NO ₂	2.0E-11	0.	0.	Atkinson et al. [1997]
HO + CO => HO ₂ + CO ₂	1.50E-13	0.	0.	De More et al. [1997]
HO + CO + M => HO ₂ + CO ₂	3.66E-33	0.	0.	De More et al. [1997]
HO + O ₃ => HO ₂	1.5E-12	0.	880	Sander et al. [2000]
HO ₂ + NO => HO + NO ₂	3.7E-12	0.	-240	Atkinson et al. [1997]
HNO ₄ + HO => NO ₂	1.3E-12	0.	-380	De More et al. [1997]
HO ₂ + O ₃ => HO	2.0E-14	0.	680	Sander et al. [2000]
NO ₃ + HO ₂ => 0.8 HO + 0.8 NO ₂ + 0.2 HNO ₃	3.5E-12	0.	0	De More et al. [1997]
NO ₃ + NO ₃ => 2 NO ₂	8.5E-13	0.	2450	De More et al. [1997]
H ₂ O ₂ + HO => HO ₂	2.9E-12	0.	160	De More et al. [1997]
HO + HO ₂ => H ₂ O + O ₂	4.80E-11	0.	-250	Sander et al. [2000]
HO + H ₂ => HO ₂	5.5E-12	0.	2000	De More et al. [1997]

(a) in molecule⁻¹.cm³.s⁻¹

(b) in K

(1) based on Atkinson et al. [1997] data assuming 20.9% of O₂ and 79.1% of N₂

Table A.2: *Photolysis reactions for inorganic species - Except mentionned, spectra and quantum yields are from SAPRC99 Carter [2000]*

Photolysis reactions	Reference
O ₃ + hν => O ³ P	Stutz et al. [2000]
O ₃ + hν => O ¹ D	
O ₂ + hν => NO + O ₃	
NO ₃ + hν => NO	
NO ₃ + hν => NO ₂ + O ₃	
HNO ₂ + hν => HO + NO	
HNO ₃ + hν => HO + NO ₂	
HNO ₄ + hν => 0.61 HO ₂ + 0.61 NO ₂ + 0.39 HO + 0.39 HNO ₃	
H ₂ O ₂ + hν => 2 HO	

Table A.3: *Fall-off reactions for inorganic species*

Fall-off reactions*	Fc	References
k_0^{300} n E/R k_∞^{300} n E/R		
$O^3P + NO (+M) \Rightarrow NO_2 (+M)$ 9.0E-32 1.5 0. 3.0E-11 0. 0.	Fc=0.6	Sander et al. [2000]
$O^3P + NO_2 (+M) \Rightarrow NO_3 (+M)$ 9.0E-32 2. 0. 2.2E-11 0. 0.	Fc=0.6	De More et al. [1997]
$NO_2 + NO_3 (+M) \Rightarrow N_2O_5 (+M)$ 2.0E-30 4.4 0. 1.4E-12 0.7 0.	Fc=0.6	Sander et al. [2000]
$N_2O_5 (+M) \Rightarrow NO_2 + NO_3 (+M)$ 6.67E-04 4.4 10991 4.67E14 0.7 10991	Fc=0.6	Sander et al. [2000]
$HO + NO (+M) \Rightarrow HNO_2 (+M)$ 7.00E-31 2.6 0. 3.60E-11 0.1 0.	Fc=0.6	De More et al. [1997]
$HO + NO_2 (+M) \Rightarrow HNO_3 (+M)$ 3.0E-30 3.0 0. 3.6E-11 0.0 0.	Fc=0.4	Troe [2001]
$HO_2 + NO_2 (+M) \Rightarrow HNO_4 (+M)$ 1.80E-31 3.2 0. 4.70E-12 0. 0.	Fc=0.6	Atkinson et al. [1997]
$HNO_4 (+M) \Rightarrow HO_2 + NO_2 (+M)$ 5.0E-6 0. 10000 2.61E15 0. 10900	Fc=0.6	Atkinson et al. [1997]
$HO + SO_2 (+M) \Rightarrow HO_2 + SULF (+M)$ 3.0E-31 3.3 0. 1.5E-12 0. 0.	Fc=0.6	De More et al. [1997]

* Parameters being used with the equation:

$$k = \frac{k_0[M]}{(1 + \frac{k_0[M]}{k_\infty})} \times Fc^{(1/[1 + \log(\frac{k_0[M]}{k_\infty})]^2)}$$

$$\text{with } k_0 = k_0^{300} \times (T/300)^{-n} \exp(-E/RT) \quad \text{and} \quad k_\infty = k_\infty^{300} \times (T/300)^{-m} \exp(-E/RT)$$

Table A.4: *Particular cases*

$\text{HO}_2 + \text{HO}_2 \Rightarrow \text{H}_2\text{O}_2$	$k = 2.3\text{E-}13 \exp(600/T)$	De More et al. [1997]
$\text{HO}_2 + \text{HO}_2 + \text{M} \Rightarrow \text{H}_2\text{O}_2$	$k = 1.7\text{E-}33 \exp(1000/T)$	De More et al. [1997]
$\text{HO}_2 + \text{HO}_2 + \text{H}_2\text{O} \Rightarrow \text{H}_2\text{O}_2$	$k = k_1 + k_2[\text{M}]$ $k_1 = 3.2\text{E-}34 \exp(2800/T)$ $k_2 = 2.38\text{E-}54 \exp(3200/T)$	De More et al. [1997]
$\text{HO} + \text{HNO}_3 \Rightarrow \text{NO}_3$	$k = k_0 + k_3[\text{M}]/(1 + k_3[\text{M}]/k_2)$	Sander et al. [2000]
	$k_0 = 2.4\text{E-}14 \exp(460/T)$	
	$k_2 = 2.7\text{E-}17 \exp(2199/T)$	
	$k_3 = 6.5\text{E-}34 \exp(1335/T)$	

Organic C1 reactions

Table A.5: *Reactions for one carbon species - Kinetic rates on the form $k=A.T^n.exp(-E_a/RT)$*

Bimolecular reactions	A (a)	n	E _a /R (b)	References and notes
CH ₄ + HO => CH ₃ O ₂	2.15E-12	0.	1735	Atkinson et al. [1999]
CH ₃ O ₂ + CH ₃ O ₂ => CH ₃ OH + CH ₂ O	6.0E-14	0.	-390	Tyndall et al. [2001]
CH ₃ O ₂ + CH ₃ O ₂ => 2 CH ₂ O + 2 HO ₂	3.5E-14	0.	-390	Tyndall et al. [2001] (1)
CH ₃ O ₂ + NO => CH ₂ O + HO ₂ + NO ₂	2.8E-12	0.	-300	Tyndall et al. [2001] (1)
CH ₃ O ₂ + NO ₃ => CH ₂ O + HO ₂ + NO ₂	1.3E-12	0.	0.	Atkinson et al. [1999]
CH ₃ O ₂ + HO ₂ => CH ₃ OOH	4.1E-13	0.	-750	Tyndall et al. [2001]
CH ₂ O + HO => CO + HO ₂	8.6E-12	0.	-20	Atkinson et al. [1999]
CH ₂ O + NO ₃ => HNO ₃ + CO + HO ₂	5.8E-16	0.	0.	
CH ₃ OOH + HO => HO + CH ₂ O	1.0E-12	0.	-190	Atkinson et al. [1999] (2)
CH ₃ OOH + HO => CH ₃ O ₂	1.9E-12	0.	-190	Atkinson et al. [1999]
HCOOH + HO => HO ₂ + CO ₂	4.5E-13	0.	0.	Atkinson et al. [1999]
CH ₃ OH + HO => CH ₂ O + HO ₂	3.1E-12	0.	360	Atkinson et al. [1999] (3)
CH ₃ OH + NO ₃ => CH ₂ O + HO ₂ + HNO ₃	9.4E-13	0.	2650	Atkinson et al. [1999]

(a) in molecule⁻¹.cm³.s⁻¹

(b) in K

Note 1 : branching ratio=0.37 for radical propagation (recommended by Tyndall et al. [2001] at 298K)

Note 2 : considering that the only way for CH₂(.)OOH is the decomposition in CH₂O + HO.

Note 3 : CH₂(.)OH => CH₂O + HO₂

Table A.6: *Photolysis reactions for one carbon species*

Photolysis reactions
HCHO + hν => CO + 2 HO ₂
HCHO + hν => H ₂ + CO
CH ₃ OOH + hν => CH ₂ O + HO ₂ + HO

Reactions for organic species

thermal reactions		A	n	Ea/R
HO + NITR01	→ 0.047 HO2 + 0.338 <1RO2_7> + 0.227 <1RO2_2> + 0.003 <1N03001#2> + 0.197 <2RO2_72> + 0.034 <1NITR01#2> + 0.045 <1NITR01#7> + 0.009 <1NONO2_7> + 0.109 <1_2NO2_2> + 0.003 <2_2NO2_72> + 0.003 CH2O + 0.196 D02000 + 0.147 D03000 + 0.460 K04000 + 0.511 N03001 + 0.070 XN2 + 0.043 OPEALC + 0.191 HNO3	0.100E-11	0.0	0
HO + NITR02	→ 0.047 HO2 + 0.338 <1RO2_7> + 0.227 <1RO2_2> + 0.003 <1N03001#2> + 0.197 <2RO2_72> + 0.034 <1NITR01#2> + 0.045 <1NITR01#7> + 0.009 <1NONO2_7> + 0.109 <1_2NO2_2> + 0.003 <2_2NO2_72> + 0.003 CH2O + 0.196 D02000 + 0.147 D03000 + 0.460 K04000 + 0.511 N03001 + 0.070 XN2 + 0.043 OPEALC + 0.191 HNO3	0.250E-10	0.0	0
HO + HP1NITR02#2	→ 0.330 HO + 0.670 <1NITR02#2>	0.293E-11	0.0	-190
HO + OPEALC	→ HO2	0.103E-10	0.0	0
HO + XN2	→ NO2	0.118E-12	0.0	0
HO2 + <1RO2_A>	→ 0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO + <1RO2_A>	→ HO2 + NO2	0.810E-11	0.0	-270
NO2 + <1RO2_A>	→ PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <1RO2_A>	→ HO2 + NO2	0.500E-11	0.0	0
<1RO2_A> + CH3O2	→ 1.380 HO2 + CH2O	0.100E-10	0.0	0
NO + <1RO2_2>	→ HO2 + NO2	0.270E-11	0.0	-360
HO2 + <1RO2_2>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1RO2_2>	→ HO2 + NO2	0.230E-11	0.0	0
<1RO2_2> + CH3O2	→ 0.880 HO2 + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
NO + <1RO2_7>	→ HO2 + NO2	0.270E-11	0.0	-360
HO2 + <1RO2_7>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1RO2_7>	→ HO2 + NO2	0.230E-11	0.0	0
HO2 + <1NONO2_A>	→ 0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO + <1NONO2_A>	→ NO2	0.810E-11	0.0	-270
NO2 + <1NONO2_A>	→ PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <1NONO2_A>	→ NO2	0.500E-11	0.0	0
<1NONO2_A> + CH3O2	→ 0.690 HO2 + CH2O	0.100E-10	0.0	0
NO + <1NONO2_2>	→ NO2	0.270E-11	0.0	-360
HO2 + <1NONO2_2>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1NONO2_2>	→ NO2	0.230E-11	0.0	0
<1NONO2_2> + CH3O2	→ 0.440 HO2 + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
NO + <1NONO2_7>	→ NO2	0.270E-11	0.0	-360
HO2 + <1NONO2_7>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1NONO2_7>	→ NO2	0.230E-11	0.0	0
NO + <1OHRO2_2>	→ HO + NO2	0.270E-11	0.0	-360
HO2 + <1OHRO2_2>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1OHRO2_2>	→ HO + NO2	0.230E-11	0.0	0
<1OHRO2_2> + CH3O2	→ 0.440 HO + 0.440 HO2 + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
HO2 + <1_2NO2_A>	→ 0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO + <1_2NO2_A>	→ 2.000 NO2	0.810E-11	0.0	-270
NO2 + <1_2NO2_A>	→ PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <1_2NO2_A>	→ 2.000 NO2	0.500E-11	0.0	0
<1_2NO2_A> + CH3O2	→ 0.690 HO2 + 0.690 NO2 + CH2O + 0.310 XN	0.100E-10	0.0	0
NO + <1_2NO2_2>	→ 2.000 NO2	0.270E-11	0.0	-360
HO2 + <1_2NO2_2>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1_2NO2_2>	→ 2.000 NO2	0.230E-11	0.0	0
<1_2NO2_2> + CH3O2	→ 0.440 HO2 + 0.440 NO2 + 0.720 CH2O + 0.280 CH3OH + 0.560 XN	0.544E-13	0.0	-945
NO + <1_2NO2_7>	→ 2.000 NO2	0.270E-11	0.0	-360
HO2 + <1_2NO2_7>	→ HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <1_2NO2_7>	→ 2.000 NO2	0.230E-11	0.0	0
HO + CA2NONO2AC	→ <2NONO2_AC>	0.698E-12	0.0	0
HO + PA2NONO2AC	→ <2NONO2_AC>	0.195E-11	0.0	-190
HO2 + <2NONO2_AC>	→ 0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO + <2NONO2_AC>	→ NO2 + CH3O2	0.810E-11	0.0	-270
NO3 + <2NONO2_AC>	→ NO2 + CH3O2	0.500E-11	0.0	0
<2NONO2_AC> + CH3O2	→ 0.690 HO2 + CH2O + 0.690 CH3O2	0.100E-10	0.0	0
HO + HP1NITR02#2	→ <1NITR02#2>	0.190E-11	0.0	-190
HO + HP1NITR02#2	→ HO	0.132E-10	0.0	0
HO + HP2RO2_22	→ <2RO2_22>	0.190E-11	0.0	-190
HO + HP2RO2_22	→ HO	0.132E-10	0.0	0
NO + <1NITR02#7>	→ NITR02	0.270E-11	0.0	-360

HO2 + <1NITR02#7>	→	HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1NITR02#7>	→	HO2 + NO2	0.230E-11	0.0	0
NO + <1N03001#2>	→	N03001	0.270E-11	0.0	-360
HO2 + <1N03001#2>	→	3.000 XC + HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1N03001#2>	→	HO2 + NO2 + 3.000 XC	0.230E-11	0.0	0
<1N03001#2> + CH3O2	→	0.880 HO2 + 3.000 XC + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
NO + <1N03001#7>	→	N03001	0.270E-11	0.0	-360
HO2 + <1N03001#7>	→	3.000 XC + HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1N03001#7>	→	HO2 + NO2 + 3.000 XC	0.230E-11	0.0	0
NO + <1NITR01#2>	→	NITR01	0.270E-11	0.0	-360
HO2 + <1NITR01#2>	→	HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1NITR01#2>	→	HO2 + NO2	0.230E-11	0.0	0
<1NITR01#2> + CH3O2	→	0.880 HO2 + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
NO + <1NITR01#7>	→	NITR01	0.270E-11	0.0	-360
HO2 + <1NITR01#7>	→	HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1NITR01#7>	→	HO2 + NO2	0.230E-11	0.0	0
NO + <1NITR02#2>	→	NITR02	0.270E-11	0.0	-360
HO2 + <1NITR02#2>	→	HP1NITR02#2	0.196E-12	0.0	-1250
NO3 + <1NITR02#2>	→	HO2 + NO2	0.230E-11	0.0	0
<1NITR02#2> + CH3O2	→	0.880 HO2 + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
HO2 + <2RO2_A2>	→	0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-945
NO + <2RO2_A2>	→	NO2 + <1RO2_2>	0.810E-11	0.0	-270
NO2 + <2RO2_A2>	→	PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <2RO2_A2>	→	NO2 + <1RO2_2>	0.500E-11	0.0	0
<2RO2_A2> + CH3O2	→	0.690 HO2 + 0.690 <1RO2_2> + CH2O	0.100E-10	0.0	0
NO + <2RO2_2A>	→	NO2 + <1RO2_A>	0.270E-11	0.0	-360
HO2 + <2RO2_2A>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2RO2_2A>	→	NO2 + <1RO2_A>	0.230E-11	0.0	0
<2RO2_2A> + CH3O2	→	0.440 HO2 + 0.440 <1RO2_A> + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-955
NO + <2RO2_22>	→	NO2 + <1RO2_2>	0.270E-11	0.0	-360
HO2 + <2RO2_22>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2RO2_22>	→	NO2 + <1RO2_2>	0.230E-11	0.0	0
<2RO2_22> + CH3O2	→	0.440 HO2 + 0.440 <1RO2_2> + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-955
NO + <2RO2_72>	→	NO2 + <1RO2_2>	0.270E-11	0.0	-360
HO2 + <2RO2_72>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2RO2_72>	→	NO2 + <1RO2_2>	0.230E-11	0.0	0
NO + <2RO2_27>	→	NO2 + <1RO2_7>	0.270E-11	0.0	-360
HO2 + <2RO2_27>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2RO2_27>	→	NO2 + <1RO2_7>	0.230E-11	0.0	0
<2RO2_27> + CH3O2	→	0.440 HO2 + 0.440 <1RO2_7> + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-955
NO + <2RO2_77>	→	NO2 + <1RO2_7>	0.270E-11	0.0	-360
HO2 + <2RO2_77>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2RO2_77>	→	NO2 + <1RO2_7>	0.230E-11	0.0	0
NO + <3RO2_727>	→	NO2 + <2RO2_27>	0.270E-11	0.0	-360
HO2 + <3RO2_727>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <3RO2_727>	→	NO2 + <2RO2_27>	0.230E-11	0.0	0
NO + <3RO2_772>	→	NO2 + <2RO2_72>	0.270E-11	0.0	-360
HO2 + <3RO2_772>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <3RO2_772>	→	NO2 + <2RO2_72>	0.230E-11	0.0	0
NO + <3RO2_722>	→	NO2 + <2RO2_22>	0.270E-11	0.0	-360
HO2 + <3RO2_722>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <3RO2_722>	→	NO2 + <2RO2_22>	0.230E-11	0.0	0
NO + <3RO2_2A2>	→	NO2 + <2RO2_A2>	0.270E-11	0.0	-360
HO2 + <3RO2_2A2>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <3RO2_2A2>	→	NO2 + <2RO2_A2>	0.230E-11	0.0	0
<3RO2_2A2> + CH3O2	→	0.440 HO2 + 0.440 <2RO2_A2> + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-955
HO2 + <2RO2_A7>	→	0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-945
NO + <2RO2_A7>	→	NO2 + <1RO2_7>	0.810E-11	0.0	-270
NO2 + <2RO2_A7>	→	PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <2RO2_A7>	→	NO2 + <1RO2_7>	0.500E-11	0.0	0
<2RO2_A7> + CH3O2	→	0.690 HO2 + 0.690 <1RO2_7> + CH2O	0.100E-10	0.0	0
HO2 + <2OHRO2_A2>	→	0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO + <2OHRO2_A2>	→	NO2 + <1OHRO2_2>	0.810E-11	0.0	-270
NO2 + <2OHRO2_A2>	→	PAN2NONO2AC	0.330E-08	-1.0	0
NO3 + <2OHRO2_A2>	→	NO2 + <1OHRO2_2>	0.500E-11	0.0	0
<2OHRO2_A2> + CH3O2	→	0.690 HO2 + 0.690 <1OHRO2_2> + CH2O	0.100E-10	0.0	0
NO + <2NONO2_7C>	→	NO2 + CH3O2	0.270E-11	0.0	-360
HO2 + <2NONO2_7C>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2NONO2_7C>	→	NO2 + CH3O2	0.230E-11	0.0	0

NO + <3NONO2_2AC>	→	NO2 + <2NONO2_AC>	0.270E-11	0.0	-360
HO2 + <3NONO2_2AC>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <3NONO2_2AC>	→	NO2 + <2NONO2_AC>	0.230E-11	0.0	0
<3NONO2_2AC> + CH3O2	→	0.440 HO2 + 0.440 <2NONO2_AC> + 0.720 CH2O + 0.280 CH3OH	0.544E-13	0.0	-945
NO + <2NONO2_2C>	→	NO2 + CH3O2	0.270E-11	0.0	-360
HO2 + <2NONO2_2C>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2NONO2_2C>	→	NO2 + CH3O2	0.230E-11	0.0	0
<2NONO2_2C> + CH3O2	→	0.440 HO2 + 0.720 CH2O + 0.280 CH3OH + 0.440 CH3O2	0.544E-13	0.0	-945
HO2 + <3NONO2_AAC>	→	0.200 O3 + 0.200 CA2NONO2AC + 0.800 PA2NONO2AC	0.640E-12	0.0	-925
NO2 + <3NONO2_AAC>	→	PAN2NONO2AC	0.330E-08	-1.0	0
NO + <3NONO2_AAC>	→	NO2 + <2NONO2_AC>	0.810E-11	0.0	-270
NO3 + <3NONO2_AAC>	→	NO2 + <2NONO2_AC>	0.500E-11	0.0	0
<3NONO2_AAC> + CH3O2	→	0.690 HO2 + 0.690 <2NONO2_AC> + CH2O	0.100E-10	0.0	0
NO + <2_2NO2_2A>	→	NO2 + <1_2NO2_A>	0.270E-11	0.0	-360
HO2 + <2_2NO2_2A>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2_2NO2_2A>	→	NO2 + <1_2NO2_A>	0.230E-11	0.0	0
<2_2NO2_2A> + CH3O2	→	0.440 HO2 + 0.440 <1_2NO2_A> + 0.720 CH2O + 0.280 CH3OH + 0.560 XN	0.544E-13	0.0	-945
NO + <2_2NO2_72>	→	NO2 + <1_2NO2_2>	0.270E-11	0.0	-360
HO2 + <2_2NO2_72>	→	HP2RO2_22	0.196E-12	0.0	-1250
NO3 + <2_2NO2_72>	→	NO2 + <1_2NO2_2>	0.230E-11	0.0	0
HO + LIMO	→	6.250 XC + 0.750 D03000 + 0.750 RO2R + 0.250 RO2N + 0.500 R2O2	0.319E-10	0.0	-500
O3 + LIMO	→	0.700 HO + 5.492 XC + 0.482 <2NONO2_AC> + 0.540 CO2 + 0.058 <2RO2_A2> + 0.058 CH2O + 0.058 D02000 + 0.482 D03000 + 0.161 RO2N + 0.539 R2O2 + 0.300 A03000	0.371E-14	0.0	870
NO3 + LIMO	→	0.750 NO2 + 6.250 XC + 0.750 D03000 + 0.250 RO2N + 0.750 R2O2 + 0.250 XN	0.122E-10	0.0	0
HO + ISO	→	0.050 <1NITR02#7> + 0.616 <1RO2_7> + 0.309 <1RO2_2> + 0.025 <1NITR02#2> + 0.924 CH2O + 0.617 MVKET + 0.308 MEACR	0.254E-10	0.0	-410
O3 + ISO	→	0.065 H2 + 0.310 HO + 0.060 HO2 + 0.011 XC + 0.469 CO + 0.366 CO2 + 0.011 <1N03001#2> + 0.239 <2RO2_2A> + 0.062 U03000 + 0.958 CH2O + 0.438 MVKET + 0.250 MEACR + 0.020 GLYOX + 0.185 HCOOH	0.786E-14	0.0	1913
NO3 + ISO	→	0.075 <1NITR02#7> + 0.740 <1_2NO2_7> + 0.185 <2NONO2_7C> + 0.740 CH2O + 0.740 MVKET + 0.075 XN2 + 0.185 NU4000	0.303E-11	0.0	446
HO + APIN	→	6.250 XC + 0.750 D03000 + 0.750 RO2R + 0.250 RO2N + 0.500 R2O2	0.121E-10	0.0	-444
O3 + APIN	→	0.700 HO + 3.873 XC + 0.051 CO + 0.298 CO2 + 0.298 <2RO2_A2> + 0.339 CH2O + 0.298 D02000 + 0.218 D03000 + 0.345 ACETO + 0.081 RO2R + 0.321 RO2N + 1.375 R2O2 + 0.300 A03000 + 0.002 GLYOX + 0.081 BIACE	0.101E-14	0.0	732
NO3 + APIN	→	0.750 NO2 + 6.250 XC + 0.750 D03000 + 0.250 RO2N + 0.750 R2O2 + 0.250 XN	0.119E-11	0.0	-490
HO + C02000	→	<1RO2_2> + D02000	0.152E-16	2.0	498
HO + C03000	→	0.703 <1RO2_7> + 0.246 <1RO2_2> + 0.006 <1N03001#2> + 0.044 <1N03001#7> + 0.246 D03000 + 0.703 ACETO	0.155E-16	2.0	61
HO + C04000	→	0.091 XC + 0.755 <1RO2_7> + 0.031 <1RO2_2> + 0.009 <1N03001#2> + 0.082 <1N03001#7> + 0.080 <2RO2_22> + 0.043 <2RO2_72> + 0.004 <1NONO2_2> + 0.086 D02000 + 0.080 D03000 + 0.031 D04000 + 0.775 K04000 + 0.020 OPEALC	0.169E-16	2.0	-145
HO + C04001	→	0.045 XC + 0.126 <1RO2_2> + 0.008 <1N03001#2> + 0.776 <2NONO2_7C> + 0.040 <1N03001#7> + 0.003 <1NONO2_2> + 0.050 <2RO2_27> + 0.053 CH2O + 0.126 D04001 + 0.825 ACETO	0.116E-16	2.0	-225
HO + C06000	→	0.259 XC + 0.108 <1RO2_7> + 0.286 <2RO2_72> + 0.006 <1NONO2_2> + 0.045 <2RO2_27> + 0.007 <1NITR01#2> + 0.217 <1NITR01#7> + 0.302 <2RO2_77> + 0.037 <1NITR02#2> + 0.076 <1NONO2_7> + 0.045 D03000 + 0.915 K04000 + 0.108 K06000 + 0.327 OPEALC	0.153E-16	2.0	-414
HO + C06001	→	0.207 XC + 0.033 <1RO2_7> + 0.001 <1RO2_2> + 0.002 <1N03001#2> + 0.012 <1N03001#7> + 0.504 <2RO2_72> + 0.045 <2RO2_27> + 0.061 <1NITR01#2> + 0.146 <1NITR01#7> + 0.193 <2RO2_77> + 0.002 <3RO2_772> + 0.002 CH2O + 0.005 D02000 + 0.624 D03000 + 0.004 D04001 + 0.269 ACETO + 0.138 K04000	0.530E-11	0.0	0
HO + C08000	→	1.233 XC + 0.105 <1NITR02#7> + 0.007 <1RO2_7> + 0.007 <2RO2_72> + 0.304 <1NITR01#7> + 0.575 <2RO2_77> + 0.002 <1NITR02#2> + 0.150 <1NONO2_7> + 0.003 C04000 + 1.164 K04000 + 0.007 K06000 + 0.582 OPEALC	0.276E-16	2.0	-378
HO + C08005	→	1.168 XC + 0.049 <1NITR02#7> + 0.015 <1RO2_7> + 0.002 <1N03001#7> + 0.095 <2RO2_72> + 0.002 <1NITR01#2> + 0.317 <1NITR01#7> + 0.472 <2RO2_77> + 0.024 <1NITR02#2> + 0.014 <3RO2_772> + 0.010 <3RO2_722> + 0.011 CH2O + 0.012 D02000 + 0.052 D03000 + 0.004 D04000 + 0.002 D04001 + 0.024 ACETO + 0.552 K04000	0.824E-11	0.0	0

HO + U02000	→	<1RO2_2> + 1.558 CH2O + 0.221 DO2000	0.196E-11	0.0	-438
O3 + U02000	→	0.130 H2 + 0.120 HO + 0.120 HO2 + 0.500 CO + 0.130 CO2 + CH2O + 0.370 HCOOH	0.914E-14	0.0	2580
NO3 + U02000	→	<1RO2_2> + ND2000	0.488E-17	2.0	2282
HO + U03000	→	0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.970 CH2O + 0.970 D02000 + 0.005 MGLYO + 0.005 OPEALC	0.485E-11	0.0	-504
O3 + U03000	→	0.065 H2 + 0.320 HO + 0.060 HO2 + 0.510 CO + 0.135 CO2 + 0.500 CH2O + 0.500 D02000 + 0.185 HCOOH + 0.170 A02000 + 0.070 CH4 + 0.260 CH3O2	0.551E-14	0.0	1878
NO3 + U03000	→	0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.025 XN2 + 0.975 NK3000	0.459E-12	0.0	1156
HO + U04000	→	0.045 XC + 0.955 <1RO2_2> + 0.045 <1N03001#2> + 0.950 CH2O + 0.950 D03000 + 0.005 K04000	0.655E-11	0.0	-467
O3 + U04000	→	0.065 H2 + 0.290 HO + 0.060 HO2 + 0.480 CO + 0.065 CO2 + 0.230 <1RO2_2> + 0.500 CH2O + 0.230 D02000 + 0.500 D03000 + 0.270 A03000 + 0.185 HCOOH	0.336E-14	0.0	1744
NO3 + U04000	→	0.045 XC + 0.925 <1RO2_2> + 0.045 <1N03001#2> + 0.030 <2RO2_22> + 0.030 D02000 + 0.231 K04000 + 0.925 N03001 + 0.045 XN2 + 0.030 ND2000	0.314E-12	0.0	938
HO + U04002	→	0.045 XC + 0.955 <1RO2_2> + 0.045 <1N03001#2> + 1.910 D02000	0.101E-10	0.0	-550
O3 + U04002	→	0.520 HO + 0.520 CO + 0.140 CO2 + D02000 + 0.340 A02000 + 0.140 CH4 + 0.520 CH3O2	0.664E-14	0.0	1059
NO3 + U04002	→	0.045 XC + 0.462 <1RO2_2> + 0.045 <1N03001#2> + 0.493 <1_2NO2_2> + 0.986 D02000 + 0.116 K04000 + 0.462 N03001 + 0.045 XN2	0.122E-17	2.0	-382
HO + U05004	→	0.858 <1RO2_7> + 0.067 <1RO2_2> + 0.005 <1NITR01#2> + 0.070 <1NITR01#7> + 0.925 CH2O + 0.925 K04000	0.610E-10	0.0	0
O3 + U05004	→	0.045 H2 + 0.692 HO + 0.042 HO2 + 0.029 XC + 0.175 CO + 0.666 CO2 + 0.029 <1N03001#2> + 0.542 <3NONO2_2AC> + 0.079 <3RO2_2A2> + 0.729 CH2O + 0.621 D02000 + 0.350 K04000 + 0.130 HCOOH	0.160E-16	0.0	0
NO3 + U05004	→	0.925 <2RO2_72> + 0.075 <1NITR01#7> + 0.925 D02000 + 0.075 XN2 + 0.925 NK3000	0.332E-12	0.0	0
HO + U05003	→	0.599 <1RO2_7> + 0.326 <1RO2_2> + 0.026 <1NITR01#2> + 0.049 <1NITR01#7> + 0.925 D02000 + 0.925 ACETO	0.192E-10	0.0	-450
O3 + U05003	→	0.856 HO + 0.156 CO + 0.725 CO2 + 0.018 <1N03001#2> + 0.683 <3NONO2_2AC> + 0.683 CH2O + 0.700 D02000 + 0.300 ACETO + 0.102 A02000 + 0.042 CH4 + 0.156 CH3O2	0.651E-14	0.0	829
NO3 + U05003	→	0.925 <1_2NO2_7> + 0.075 <1NITR01#7> + 0.925 D02000 + 0.925 ACETO + 0.075 XN2	0.937E-11	0.0	0
HO + BUTYN	→	0.670 HO + 0.330 <2NONO2_AC> + 0.330 CO2 + 0.670 BIACE + 0.330 A02000	0.100E-10	0.0	-300
O3 + BUTYN	→	HO + -0.080 XC + 0.961 CO2 + 0.961 <2RO2_A2> + 0.961 CH2O + 0.961 D02000 + 0.039 RO2N + 0.961 R2O2	0.100E-13	0.0	3915
HO + ACTYN	→	0.603 HO + 0.297 HO2 + 0.393 CO + 0.096 CH2O + 0.100 RO2R + 0.607 GLYOX + 0.297 HCOOH	0.940E-11	0.0	700
HO + ACTYN	→	0.500 HO + 1.500 HO2 + 1.500 CO + 0.500 CO2	0.200E-13	0.0	4398
HO + BENZ	→	0.236 HO2 + 1.114 XC + 0.764 RO2R + 0.207 GLYOX + 0.236 PHEN + 0.764 DCB1	0.247E-11	0.0	207
HO + TOL	→	0.234 HO2 + 1.177 XC + 0.085 BALD + 0.758 RO2R + 0.008 RO2N + 0.116 GLYOX + 0.135 MGLYO + 0.460 DCB1 + 0.234 CRES + 0.156 DCB2 + 0.057 DCB3	0.181E-11	0.0	-355
HO + ETBNZ	→	0.190 HO2 + 2.340 XC + 0.786 RO2R + 0.024 RO2N + 0.094 GLYOX + 0.239 K06000 + 0.109 MGLYO + 0.498 DCB1 + 0.190 CRES + 0.049 DCB3	0.710E-11	0.0	0
HO + T124B	→	0.186 HO2 + 2.729 XC + 0.044 BALD + 0.804 RO2R + 0.010 RO2N + 0.063 GLYOX + 0.079 BIACE + 0.364 MGLYO + 0.733 DCB1 + 0.186 CRES + 0.027 DCB3	0.325E-10	0.0	0
HO + D02000	→	<2NONO2_AC> + CO2	0.560E-11	0.0	-310
NO3 + D02000	→	<2NONO2_AC> + CO2 + HNO3	0.140E-11	0.0	1860
HO + D03000	→	CO2 + <2RO2_A2> + D02000	0.200E-10	0.0	0
NO3 + D03000	→	CO2 + <2RO2_A2> + D02000 + HNO3	0.600E-14	0.0	0
HO + D04000	→	0.006 XC + 0.014 CO + 0.862 CO2 + 0.840 <2RO2_A2> + 0.117 <1RO2_7> + 0.022 <1N03001#2> + 0.006 <1N03001#7> + 0.015 <2RO2_72> + 0.022 <1NONO2_A> + 0.014 CH2O + 0.015 D02000 + 0.957 D03000 + 0.029 K04000 + 0.001 GLYOX	0.526E-11	0.0	-446
NO3 + D04000	→	CO2 + 0.975 <2RO2_A2> + 0.025 <1N03001#2> + 0.025 <1NONO2_A> + 0.975 D03000 + HNO3	0.117E-13	0.0	0
HO + D04001	→	0.003 XC + 0.057 CO + 0.940 CO2 + 0.057 <1RO2_7> + 0.058 <1N03001#7> + 0.055 <1NONO2_A> + 0.884 <2RO2_A7> + 0.942 ACETO	0.661E-11	0.0	-411

NO3 + D04001	→	CO2 + 0.059 <1N03001#7> + 0.059 <1NONO2_A> + 0.941 <2RO2_A7> + 0.941 ACETO + HNO3	0.124E-13	0.0	0
HO + BALD	→	BZCOO2	0.129E-10	0.0	0
NO3 + BALD	→	HNO3 + BZCOO2	0.140E-11	0.0	1872
HO + ACETO	→	0.975 CO2 + 0.025 <1N03001#2> + 0.975 <3NONO2_2AC> + 0.975 CH2O	0.211E-17	2.0	-10
HO + K04000	→	0.045 XC + 0.575 CO2 + 0.380 <1RO2_2> + 0.045 <1N03001#2> + 0.506 <3NONO2_2AC> + 0.069 <3RO2_2A2> + 0.069 CH2O + 0.575 D02000 + 0.380 D03000 + 0.095 K04000	0.253E-17	2.0	-503
HO + K06001	→	0.114 XC + 0.866 CO2 + 0.020 <1N03001#2> + 0.011 <1NITR01#2> + 0.103 <1NITR01#7> + 0.804 <1NONO2_7> + 0.866 <3NONO2_2AC> + 0.784 CH2O + 0.082 D04001 + 0.804 ACETO	0.759E-12	0.0	-834
HO + O02000	→	HO2 + D02000	0.410E-11	0.0	70
HO + EK3000	→	0.865 CO + 0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.865 A02000 + 0.110 ED3000	0.530E-12	0.0	128
HO + EK4000	→	0.045 XC + 0.805 CO2 + 0.151 <1RO2_2> + 0.045 <1N03001#2> + 0.770 <3NONO2_2AC> + 0.035 <2NONO2_2C> + 0.035 D02000 + 0.090 D03000 + 0.083 K04000 + 0.770 A02000	0.160E-11	0.0	0
HO + EK5001	→	0.853 CO2 + 0.071 <1RO2_2> + 0.845 <2NONO2_7C> + 0.001 <2RO2_22> + 0.008 <1NONO2_2> + 0.006 <1NITR01#2> + 0.069 <1NITR01#7> + 0.008 <3NONO2_2AC> + 0.009 CH2O + 0.071 D03000 + 0.845 ACETO + 0.036 K04000 + 0.008 A02000	0.301E-12	0.0	-770
HO + EK6000	→	0.131 XC + 0.223 CO2 + 0.463 <1RO2_7> + 0.018 <1RO2_2> + 0.007 <1N03001#2> + 0.116 <2RO2_22> + 0.048 <2RO2_72> + 0.048 <1NITR01#2> + 0.066 <1NITR01#7> + 0.015 <1NITR02#2> + 0.002 <1NONO2_7> + 0.206 <3RO2_2A2> + 0.012 <2NONO2_2C> + 0.009 C04000 + 0.050 D02000 + 0.370 D03000 + 0.012 D04000 + 0.465 K04000 + 0.463 EK3000	0.210E-11	0.0	-299
NO + RO2R	→	HO2 + NO2	0.270E-11	0.0	-360
HO2 + RO2R	→	-3.000 XC + H03000	0.264E-12	0.0	-1250
NO3 + RO2R	→	HO2 + NO2	0.230E-11	0.0	0
RO2R + CH3O2	→	0.680 HO2 + 0.670 CH2O + 0.330 CH3OH	0.282E-13	0.0	-845
NO + RO2N	→	0.250 C04000 + N05001	0.270E-11	0.0	-360
HO2 + RO2N	→	3.000 XC + H03000	0.264E-12	0.0	-1250
NO3 + RO2N	→	HO2 + NO2 + 2.000 XC + K04000	0.230E-11	0.0	0
RO2N + CH3O2	→	0.680 HO2 + 0.680 XC + 0.670 CH2O + 0.340 K04000 + 0.330 CH3OH + 0.660 K06000	0.282E-13	0.0	-845
NO + R2O2	→	NO2	0.270E-11	0.0	-360
HO2 + R2O2	→	HO2	0.264E-12	0.0	-1250
NO3 + R2O2	→	NO2	0.230E-11	0.0	0
R2O2 + CH3O2	→	CH3O2	0.282E-13	0.0	-845
HO + A03000	→	0.410 CO + 0.448 CO2 + 0.576 <1RO2_2> + 0.014 <1N03001#2> + 0.410 <1OHRO2_2> + 0.859 D02000 + 0.128 AD3000	0.120E-11	0.0	0
HO + MVKET	→	0.045 XC + 0.764 CO2 + 0.191 <1RO2_2> + 0.045 <1N03001#2> + 0.764 <3NONO2_2AC> + 0.190 CH2O + 0.764 D02000 + 0.191 MGLYO + 0.001 OPEALC	0.267E-11	0.0	-612
O3 + MVKET	→	0.123 H2 + 0.164 HO + 0.114 HO2 + 0.050 <2NONO2_AC> + 0.525 CO + 0.174 CO2 + 0.050 CH2O + 0.352 HCOOH + 0.950 MGLYO	0.890E-15	0.0	1521
NO3 + MVKET	→	0.045 XC + 0.955 CO2 + 0.045 <1N03001#2> + 0.955 <3NONO2_2AC> + 0.045 XN2 + 0.955 ND2000	0.120E-15	0.0	0
HO + MEACR	→	0.022 XC + 0.338 CO + 1.027 CO2 + 0.372 <1RO2_7> + 0.093 <1RO2_2> + 0.004 <1N03001#2> + 0.018 <1N03001#7> + 0.513 <3NONO2_AAC> + 0.640 CH2O + 0.465 MGLYO + 0.338 OPEALC	0.773E-11	0.0	-379
O3 + MEACR	→	0.117 H2 + 0.208 HO + 0.108 HO2 + 0.100 <2NONO2_AC> + 0.550 CO + 0.217 CO2 + 0.100 CH2O + 0.333 HCOOH + 0.900 MGLYO	0.136E-14	0.0	2112
NO3 + MEACR	→	0.018 XC + 0.373 CO + 1.220 CO2 + 0.373 <1RO2_7> + 0.018 <1N03001#7> + 0.610 <3NONO2_AAC> + 0.610 CH2O + 0.018 XN2 + 0.373 NK3000 + 0.610 HNO3	0.134E-11	0.0	1726
HO + N03001	→	0.738 HO2 + 0.145 NO2 + 0.112 <1RO2_2> + 0.003 <1N03001#2> + 0.003 <1_2NO2_2> + 0.003 CH2O + 0.003 D02000 + 0.882 ACETO + 0.003 XN2 + 0.738 HNO3 + 0.112 N03002	0.620E-12	0.0	230
HO + GLYOX	→	0.700 HO2 + 1.700 CO + 0.300 CO2 + 0.300 <1RO2_A>	0.110E-10	0.0	0
NO3 + GLYOX	→	0.700 HO2 + 1.700 CO + 0.300 CO2 + 0.300 <1RO2_A> + HNO3	0.280E-11	0.0	2375
HO + NU4000	→	0.045 XC + 0.764 CO2 + 0.191 <1RO2_2> + 0.045 <1N03001#2> + 0.764 <2_2NO2_2A> + 0.954 CH2O + 0.001 N03001 + 0.045 XN2 + 0.764 D02000 + 0.190 ND3000	0.241E-10	0.0	0
O3 + NU4000	→	0.123 H2 + 0.164 HO + 0.114 HO2 + 0.525 CO + 0.174 CO2 + 0.050 <1_2NO2_A> + 0.100 CH2O + 0.352 HCOOH + 0.950 ND3000	0.539E-17	0.0	0
NO3 + NU4000	→	0.045 XC + 0.955 CO2 + 0.045 <1N03001#2> + 0.955 <2_2NO2_2A> + 0.955 CH2O + 0.090 XN2 + 0.955 ND2000	0.120E-15	0.0	0

HO + BIACE	→	0.045 XC + 0.955 CO + 0.955 CO ₂ + 0.045 <1N03001#2> + 0.955 <3NONO2_2AC> + 0.955 CH ₂ O	0.140E-17	2.0	-194
HO + K06000	→	0.115 XC + 0.179 CO ₂ + 0.561 <1RO2_7> + 0.003 <1N03001#2> + 0.143 <2RO2_72> + 0.015 <1NITR01#2> + 0.099 <1NITR01#7> + 0.070 <1NONO2_7> + 0.180 <3NONO2_2AC> + 0.561 C04000 + 0.067 CH ₂ O + 0.144 D02000 + 0.211 D03000 + 0.113 D04000 + 1.157 K04000	0.910E-11	0.0	0
HO + D02000	→	0.097 HO ₂ + 0.904 CO ₂ + 0.904 <1RO2_A> + 0.904 CH ₂ O + 0.097 GLYOX	0.100E-10	0.0	0
NO ₃ + D02000	→	CO ₂ + <1RO2_A> + CH ₂ O + HNO ₃	0.120E-13	0.0	0
HO + ND2000	→	0.077 HO ₂ + 0.071 CO + 0.923 CO ₂ + 0.923 <1_2NO2_A> + 0.994 CH ₂ O + 0.006 GLYOX + 0.077 HNO ₃	0.454E-11	0.0	0
NO ₃ + ND2000	→	CO ₂ + <1_2NO2_A> + CH ₂ O + HNO ₃	0.120E-13	0.0	0
HO + MGLYO	→	<2NONO2_AC> + CO + CO ₂	0.840E-12	0.0	-830
NO ₃ + MGLYO	→	<2NONO2_AC> + CO + CO ₂ + HNO ₃	0.240E-14	0.0	0
HO + A02000	→	0.113 CO + 0.886 CO ₂ + 0.001 <1RO2_2> + 0.113 <1OHRO2_2> + 0.113 CH ₂ O + 0.886 CH ₃ O ₂ + 0.001 AD2000	0.800E-12	0.0	0
HO + NK3000	→	0.050 NO ₂ + 0.758 <2NONO2_AC> + 0.945 CO ₂ + 0.005 <1N03001#2> + 0.187 <2_2NO2_2A> + 1.132 CH ₂ O + 0.005 XN ₂ + 0.050 MGLYO + 0.758 HNO ₃	0.490E-12	0.0	0
HO + PHEN	→	4.100 XC + 0.760 RO ₂ R + 0.230 GLYOX + 0.240 BZO	0.263E-10	0.0	0
NO ₃ + PHEN	→	HNO ₃ + BZO	0.378E-11	0.0	0
HO + DCB1	→	CO + D03000 + RO ₂ R	0.500E-10	0.0	0
O ₃ + DCB1	→	0.500 HO + 1.500 HO ₂ + 1.500 CO + 0.500 CO ₂ + GLYOX	0.200E-17	0.0	0
HO + CRES	→	4.870 XC + 0.760 RO ₂ R + 0.230 MGLYO + 0.240 BZO	0.420E-10	0.0	0
NO ₃ + CRES	→	XC + HNO ₃ + BZO	0.137E-10	0.0	0
HO + DCB2	→	<2NONO2_AC> + CO ₂ + D03000 + R ₂ O ₂	0.500E-10	0.0	0
HO + DCB3	→	<2NONO2_AC> + CO ₂ + D03000 + R ₂ O ₂	0.500E-10	0.0	0
NO ₂ + BZCOO2	→	PBZN	0.330E-08	-1.0	0
NO + BZCOO2	→	NO ₂ + CO ₂ + R ₂ O ₂ + BZO	0.810E-11	0.0	-270
HO ₂ + BZCOO2	→	0.800 O ₃ + 4.000 XC + 0.200 A03000 + 0.800 G03000	0.640E-12	0.0	-925
NO ₃ + BZCOO2	→	NO ₂ + CO ₂ + R ₂ O ₂ + BZO	0.500E-11	0.0	0
CH ₃ O ₂ + BZCOO2	→	0.680 HO ₂ + 1.280 XC + 0.680 CO ₂ + CH ₂ O + 0.680 R ₂ O ₂ + 0.320 A03000 + 0.680 BZO	0.100E-10	0.0	0
HO + ED3000	→	0.975 CO + 0.975 CO ₂ + 0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.975 CH ₂ O	0.422E-13	0.0	0
NO ₃ + ED3000	→	<2NONO2_AC> + 2.000 CO ₂ + HNO ₃	0.120E-13	0.0	0
HO + H03000	→	0.781 HO + 0.209 <1RO2_2> + 0.005 <1N03001#2> + 0.005 <1OHRO2_2> + 0.005 CH ₂ O + 0.005 D02000 + 0.945 D03000 + 0.045 HK3000	0.220E-10	0.0	0
HO + N05001	→	0.047 HO ₂ + 0.338 <1RO2_7> + 0.227 <1RO2_2> + 0.003 <1N03001#2> + 0.197 <2RO2_72> + 0.034 <1NITR01#2> + 0.045 <1NITR01#7> + 0.009 <1NONO2_7> + 0.109 <1_2NO2_2> + 0.003 <2_2NO2_72> + 0.003 CH ₂ O + 0.196 D02000 + 0.147 D03000 + 0.460 K04000 + 0.511 N03001 + 0.070 XN ₂ + 0.043 OPEALC + 0.191 HNO ₃	0.185E-11	0.0	0
HO + AD3000	→	0.992 CO + CO ₂ + 0.008 <2RO2_A2> + 0.992 <2OHRO2_A2> + 0.992 CH ₂ O + 0.008 AD2000	0.216E-10	0.0	0
NO ₃ + AD3000	→	0.992 CO + CO ₂ + 0.008 <2RO2_A2> + 0.992 <2OHRO2_A2> + 0.992 CH ₂ O + HNO ₃ + 0.008 AD2000	0.120E-13	0.0	0
HO + N03002	→	0.077 HO ₂ + 0.077 CO + 0.923 CO ₂ + 0.923 <1_2NO2_A> + D02000 + 0.077 HNO ₃	0.459E-11	0.0	0
NO ₃ + N03002	→	CO ₂ + <1_2NO2_A> + D02000 + HNO ₃	0.120E-13	0.0	0
HO + ND3000	→	CO + CO ₂ + <1_2NO2_A> + CH ₂ O	0.130E-10	0.0	0
NO ₃ + ND3000	→	CO + CO ₂ + <1_2NO2_A> + CH ₂ O + HNO ₃	0.240E-14	0.0	0
HO + NU3000	→	0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.966 CH ₂ O + 0.034 XN ₂ + 0.966 ND2000 + 0.009 MGLYO + 0.009 OPEALC	0.347E-10	0.0	0
O ₃ + NU3000	→	0.065 H ₂ + 0.320 HO + 0.060 HO ₂ + 0.330 NO ₂ + 0.510 CO + 0.135 CO ₂ + 0.830 CH ₂ O + 0.185 HCOOH + 0.500 ND2000 + 0.170 AN2000	0.101E-16	0.0	0
NO ₃ + NU3000	→	0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.050 XN ₂ + 0.975 NN3001	0.135E-13	0.0	0
HO + AD2000	→	HO + 2.000 CO	0.986E-11	0.0	0
NO ₃ + AD2000	→	HO + 2.000 CO + HNO ₃	0.240E-14	0.0	0
NO ₂ + BZO	→	NPHE	0.230E-10	0.0	-151
HO ₂ + BZO	→	PHEN	0.190E-12	0.0	-1298
BZO	→	PHEN	0.100E-02	0.0	0
PBZN	→	NO ₂ + BZCOO2	0.790E+17	0.0	14000
HO + G03000	→	0.150 CO + 0.846 CO ₂ + 0.846 <2RO2_A2> + 0.150 <1RO2_2> + 0.004 <1N03001#2> + 0.996 D02000	0.449E-11	0.0	0
HO + HK3000	→	0.736 HO + 0.258 CO ₂ + 0.007 <1N03001#2> + 0.258 <3NONO2_2AC> + 0.258 CH ₂ O + 0.736 MGLYO	0.140E-10	0.0	0
HO + AN2000	→	0.406 HO + 0.003 HO ₂ + 0.591 NO ₂ + 0.406 CO + 0.591 CO ₂ + 0.997 CH ₂ O + 0.409 HNO ₃ + 0.003 AD2000	0.897E-12	0.0	0

HO + NN3001	→	0.062 NO2 + 0.938 CO2 + 0.938 <1_2NO2_A> + 1.876 CH2O + 0.938 HNO3 + 0.062 ND3000	0.776E-12	0.0	0
HO + ACROL	→	0.863 CO + 0.674 CO2 + 0.318 <1RO2_2> + 0.008 <1N03001#2> + 0.674 <1RO2_A> + 0.688 CH2O + 0.126 GLYOX + 0.245 DO2000 + 0.002 DK3000	0.655E-11	0.0	-333
O3 + ACROL	→	0.123 H2 + 0.139 HO + 0.189 HO2 + 0.550 CO + 0.148 CO2 + 0.050 CH2O + 0.950 GLYOX + 0.352 HCOOH	0.136E-14	0.0	2519
NO3 + ACROL	→	0.917 CO + CO2 + <1RO2_A> + 0.917 CH2O + 0.083 GLYOX + HNO3	0.250E-14	0.0	0
NO3 + NPHE	→	HNO3 + BZNO2O	0.378E-11	0.0	0
HO + DK3000	→	0.151 HO2 + 0.849 CO + 0.849 CO2 + 0.849 <1RO2_A> + 0.849 CH2O + 0.151 DD3002	0.152E-10	0.0	0
NO3 + DK3000	→	CO + CO2 + <1RO2_A> + CH2O + HNO3	0.240E-14	0.0	0
NO2 + BZNO2O	→	6.000 XC + 2.000 XN	0.230E-10	0.0	-151
HO2 + BZNO2O	→	NPHE	0.190E-12	0.0	-1298
BZNO2O	→	NPHE	0.100E-02	0.0	0
HO + DD3002	→	2.000 CO + CO2 + <1RO2_A>	0.253E-10	0.0	0
NO3 + DD3002	→	2.000 CO + CO2 + <1RO2_A> + HNO3	0.480E-14	0.0	0

peroxy permutation reactions			A	n	Ea/R
<1RO2_A> + C_PERO2	→	0.750 HO2	0.100E-10	0.0	0
<1RO2_A> + C_PERO9	→	HO2	0.500E-11	0.0	-500
<1RO2_2> + C_PERO2	→	0.500 HO2	0.156E-13	0.0	-1500
<1RO2_2> + C_PERO9	→	0.750 HO2	0.100E-10	0.0	0
<1NONO2_A> + C_PERO2	→		0.100E-10	0.0	0
<1NONO2_A> + C_PERO9	→		0.500E-11	0.0	-500
<1NONO2_2> + C_PERO2	→		0.156E-13	0.0	-1500
<1NONO2_2> + C_PERO9	→		0.100E-10	0.0	0
<1OHRO2_2> + C_PERO2	→	0.500 HO	0.156E-13	0.0	-1500
<1OHRO2_2> + C_PERO9	→	0.750 HO	0.100E-10	0.0	0
<1_2NO2_A> + C_PERO2	→	0.750 NO2 + 0.250 XN	0.100E-10	0.0	0
<1_2NO2_A> + C_PERO9	→	NO2	0.500E-11	0.0	-500
<1_2NO2_2> + C_PERO2	→	0.500 NO2 + 0.500 XN	0.156E-13	0.0	-1500
<1_2NO2_2> + C_PERO9	→	0.750 NO2 + 0.250 XN	0.100E-10	0.0	0
<2NONO2_AC> + C_PERO2	→	0.750 CH3O2	0.100E-10	0.0	0
<2NONO2_AC> + C_PERO9	→	CH3O2	0.500E-11	0.0	-500
<1N03001#2> + C_PERO2	→	0.500 HO2 + 3.000 XC	0.156E-13	0.0	-1500
<1N03001#2> + C_PERO9	→	0.750 HO2 + 3.000 XC	0.100E-10	0.0	0
<1NITR01#2> + C_PERO2	→	0.500 HO2	0.156E-13	0.0	-1500
<1NITR01#2> + C_PERO9	→	0.750 HO2	0.100E-10	0.0	0
<1NITR02#2> + C_PERO2	→	0.500 HO2	0.156E-13	0.0	-1500
<1NITR02#2> + C_PERO9	→	0.750 HO2	0.100E-10	0.0	0
<2RO2_A2> + C_PERO2	→	0.750 <1RO2_2>	0.100E-10	0.0	0
<2RO2_A2> + C_PERO9	→	<1RO2_2>	0.500E-11	0.0	-500
<2RO2_2A> + C_PERO2	→	0.500 <1RO2_A>	0.156E-13	0.0	-1500
<2RO2_2A> + C_PERO9	→	0.750 <1RO2_A>	0.100E-10	0.0	0
<2RO2_22> + C_PERO2	→	0.500 <1RO2_2>	0.156E-13	0.0	-1500
<2RO2_22> + C_PERO9	→	0.750 <1RO2_2>	0.100E-10	0.0	0
<2RO2_27> + C_PERO2	→	0.500 <1RO2_7>	0.156E-13	0.0	-1500
<2RO2_27> + C_PERO9	→	0.750 <1RO2_7>	0.100E-10	0.0	0
<3RO2_2A2> + C_PERO2	→	0.500 <2RO2_A2>	0.156E-13	0.0	-1500
<3RO2_2A2> + C_PERO9	→	0.750 <2RO2_A2>	0.100E-10	0.0	0
<2RO2_A7> + C_PERO2	→	0.750 <1RO2_7>	0.100E-10	0.0	0
<2RO2_A7> + C_PERO9	→	<1RO2_7>	0.500E-11	0.0	-500
<2OHRO2_A2> + C_PERO2	→	0.750 <1OHRO2_2>	0.100E-10	0.0	0
<2OHRO2_A2> + C_PERO9	→	<1OHRO2_2>	0.500E-11	0.0	-500
<3NONO2_2AC> + C_PERO2	→	0.500 <2NONO2_AC>	0.156E-13	0.0	-1500
<3NONO2_2AC> + C_PERO9	→	0.750 <2NONO2_AC>	0.100E-10	0.0	0
<2NONO2_2C> + C_PERO2	→	0.500 CH3O2	0.156E-13	0.0	-1500
<2NONO2_2C> + C_PERO9	→	0.750 CH3O2	0.100E-10	0.0	0
<3NONO2_AAC> + C_PERO2	→	0.750 <2NONO2_AC>	0.100E-10	0.0	0
<3NONO2_AAC> + C_PERO9	→	<2NONO2_AC>	0.500E-11	0.0	-500
<2_2NO2_2A> + C_PERO2	→	0.500 <1_2NO2_A> + 0.500 XN	0.156E-13	0.0	-1500
<2_2NO2_2A> + C_PERO9	→	0.750 <1_2NO2_A> + 0.250 XN	0.100E-10	0.0	0
RO2R + C_PERO2	→	0.400 HO2	0.162E-13	0.0	-1400
RO2R + C_PERO9	→	0.650 HO2	0.100E-10	0.0	0
RO2N + C_PERO2	→	0.400 HO2 + 0.800 XC + 0.400 K04000 + 0.600 K06000	0.162E-13	0.0	-1400
RO2N + C_PERO9	→	0.650 HO2 + 1.300 XC + 0.650 K04000 + 0.350 K06000	0.100E-10	0.0	0
R2O2 + C_PERO2	→		0.162E-13	0.0	-1400
R2O2 + C_PERO9	→		0.100E-10	0.0	0

BZCOO2 + C_PERO2	→	XC + 0.750 CO2 + 0.750 R2O2 + 0.250 A03000 + 0.750 BZO	0.100E-10	0.0	0
BZCOO2 + C_PERO9	→	CO2 + R2O2 + BZO	0.500E-11	0.0	-500
fall-off reactions					
PAN2NONO2AC (+M)	→	NO2 + <2NONO2_AC>(+M)			
k ₀ = 0.190E-02 exp(-12175/T)					
k _∞ = 0.280E+17 exp(-13580/T)					
Fc= 0.6					
NO2 + <2NONO2_AC> (+M)	→	PAN2NONO2AC(+M)			
k ₀ = 0.850E-28 (T/300) ^{6.5}					
k _∞ = 0.110E-10 (T/300) ^{1.0}					
Fc= 0.6					
photolytic reactions			label	factor	
NITR01 + HV	→	0.244 HO2 + NO2 + 0.699 <1RO2_2> + 0.057 <1NITR01#2> + 0.061 C04000 + 1.118 K04000 + 0.175 OPEALC	900	1.0	
NITR02 + HV	→	0.244 HO2 + NO2 + 0.699 <1RO2_2> + 0.057 <1NITR01#2> + 0.061 C04000 + 1.118 K04000 + 0.175 OPEALC	900	1.0	
XN2 + HV	→	HO2 + NO2	900	1.0	
PAN2NONO2AC + HV	→	NO2 + <2NONO2_AC>	1400	1.0	
PA2NONO2AC + HV	→	HO + <2NONO2_AC>	40100	1.0	
HP1NITR02#2 + HV	→	HO + HO2	40100	1.0	
HP2RO2_22 + HV	→	HO + HO2	40100	1.0	
D02000 + HV	→	HO2 + CO + CH3O2	1700	1.0	
D03000 + HV	→	HO2 + CO + <1RO2_2> + D02000	1800	1.0	
D04000 + HV	→	HO2 + CO + 0.975 <1RO2_2> + 0.025 <1N03001#2> + 0.975 D03000	1900	1.0	
D04000 + HV	→	U02000 + D02000	2000	1.0	
D04001 + HV	→	HO2 + CO + 0.941 <1RO2_7> + 0.059 <1N03001#7> + 0.941 ACETO	2100	1.0	
BALD + HV	→	7.000 XC	14	1.0	
ACETO + HV	→	<2NONO2_AC> + CO2 + CH3O2	3000	1.0	
K04000 + HV	→	<2NONO2_AC> + CO2 + <1RO2_2> + D02000	3100	1.0	
K04000 + HV	→	CO2 + <2RO2_A2> + D02000 + CH3O2	3200	1.0	
K06001 + HV	→	0.045 XC + <2NONO2_AC> + CO2 + 0.673 <1RO2_2> + 0.045 <1N03001#2> + 0.017 <1N03001#7> + 0.017 <1NONO2_2> + 0.265 <2RO2_27> + 0.282 CH2O + 0.673 D04001 + 0.265 ACETO	3600	1.0	
K06001 + HV	→	U03000 + ACETO	3700	1.0	
MVKET + HV	→	CO + U03000	4900	1.0	
MVKET + HV	→	HO2 + <2NONO2_AC> + 0.917 CO + CO2 + 0.917 CH2O + 0.083 GLYOX	5000	1.0	
MEACR + HV	→	HO2 + <2NONO2_AC> + CO + CO2 + CH2O	4300	1.0	
MEACR + HV	→	HO + CO + 0.975 CO2 + 0.025 <1N03001#2> + 0.975 <3NONO2_2AC> + 0.975 CH2O	4400	1.0	
MEACR + HV	→	HO2 + 2.000 CO2 + <3NONO2_AAC> + CH2O	4500	1.0	
N03001 + HV	→	HO2 + NO2 + ACETO	400	1.0	
GLYOX + HV	→	H2 + 2.000 CO	5100	1.0	
GLYOX + HV	→	2.000 HO2 + 2.000 CO	5200	1.0	
GLYOX + HV	→	CO + CH2O	5300	1.0	
NU4000 + HV	→	NO2 + 0.917 CO + CO2 + <1RO2_A> + 1.917 CH2O + 0.083 GLYOX	10100	1.0	
NU4000 + HV	→	HO2 + 0.917 CO + CO2 + <1_2NO2_A> + 1.917 CH2O + 0.083 GLYOX	31700	1.0	
NU4000 + HV	→	CO + NU3000	31600	1.0	
BIACE + HV	→	2.000 <2NONO2_AC> + 2.000 CO2	5700	1.0	
K06000 + HV	→	0.076 XC + <2NONO2_AC> + CO2 + 0.261 <1RO2_2> + 0.076 <1N03001#2> + 0.663 <2RO2_22> + 0.031 <1NONO2_2> + 0.663 D03000 + 0.261 D04000 + 0.166 K04000 + 0.166 OPEALC	30200	1.0	
K06000 + HV	→	U03000 + ACETO	30300	1.0	
DO2000 + HV	→	2.000 HO2 + CO + CH2O	7400	1.0	
ND2000 + HV	→	HO2 + NO2 + 0.917 CO + 0.917 CH2O + 0.083 GLYOX	10100	1.0	
ND2000 + HV	→	HO2 + NO2 + CO + CH2O	20300	1.0	
MGLYO + HV	→	HO2 + <2NONO2_AC> + CO + CO2	5400	1.0	
MGLYO + HV	→	CO + D02000	5500	2.0	
MGLYO + HV	→	2.000 CO + CH4	5600	1.0	
NK3000 + HV	→	CO2 + <1_2NO2_A> + CH2O + CH3O2	30100	1.0	
NK3000 + HV	→	NO2 + <2NONO2_AC> + CO2 + CH2O	10100	1.0	
DCB2 + HV	→	0.500 HO2 + 0.500 XC + 0.500 <2NONO2_AC> + CO + 0.500 CO2 + RO2R + R2O2 + 0.500 GLYOX + 0.500 MGLYO	12	1.0	
DCB3 + HV	→	0.500 HO2 + 0.500 XC + 0.500 <2NONO2_AC> + CO + 0.500 CO2 + RO2R + R2O2 + 0.500 GLYOX + 0.500 MGLYO	13	1.0	
H03000 + HV	→	HO + HO2 + D03000	40100	1.0	

N05001 + HV	→	0.244 HO2 + NO2 + 0.699 <1RO2_2> + 0.057 <1NITR01#2> + 0.061 C04000 + 1.118 K04000 + 0.175 OPEALC	900	1.0
AD3000 + HV	→	HO2 + 1.992 CO + 0.008 <1RO2_2> + 0.992 <1OHRO2_2> + 0.992 CH2O + 0.008 AD2000	20300	1.0
N03002 + HV	→	HO2 + NO2 + 0.995 CO + 0.995 D02000 + 0.005 MGLYO	10200	1.0
N03002 + HV	→	HO2 + NO2 + CO + D02000	20300	1.0
ND3000 + HV	→	NO2 + CO + CO2 + <1RO2_A> + CH2O	10100	1.0
ND3000 + HV	→	HO2 + CO + CO2 + <1_2NO2_A> + CH2O	21400	1.0
ND3000 + HV	→	CO + ND2000	21500	2.0
NU3000 + HV	→	HO2 + NO2 + ACROL	10100	1.0
AD2000 + HV	→	CO2 + CH2O	7800	1.0
AD2000 + HV	→	2.000 CO	7900	1.0
G03000 + HV	→	HO + CO2 + <1RO2_2> + D02000	40100	1.0
HK3000 + HV	→	HO + <2NONO2_AC> + CO2 + CH2O	31900	1.0
HK3000 + HV	→	HO + <2NONO2_AC> + CO2 + CH2O	40100	1.0
AN2000 + HV	→	0.992 HO + 0.008 HO2 + NO2 + 0.992 CO + 0.992 CH2O + 0.008 AD2000	10100	1.0
NN3001 + HV	→	NO2 + CO2 + <1_2NO2_A> + 2.000 CH2O	10100	2.0
NN3001 + HV	→	NO2 + CO2 + <1_2NO2_A> + 2.000 CH2O	30100	1.0
ACROL + HV	→	HO2 + 0.917 CO + CO2 + <1RO2_A> + 0.917 CH2O + 0.083 GLYOX	4000	1.0
ACROL + HV	→	2.000 HO2 + 1.917 CO + 0.917 CH2O + 0.083 GLYOX	4100	1.0
ACROL + HV	→	0.520 HO + 1.520 CO + 0.140 CO2 + 0.340 A02000 + 0.140 CH4 + 0.520 CH3O2	4200	1.0
DK3000 + HV	→	HO2 + CO + CO2 + <1RO2_A> + CH2O	21400	1.0
DK3000 + HV	→	CO + D02000	21500	1.0
DK3000 + HV	→	2.000 CO + CH3OH	21600	1.0
DD3002 + HV	→	HO2 + 2.000 CO + CO2 + <1RO2_A>	21400	2.0
DD3002 + HV	→	CO + GLYOX	21500	2.0
DD3002 + HV	→	2.000 CO + CH2O	21600	2.0

Reference compounds and reaction types used to assign photolysis parameters for each label

Reference compound	Label	Photolysis pathway
DCB2	12	DCB2 \rightarrow product (see SAPRC99 reactions)
DCB3	13	DCB3 \rightarrow product (see SAPRC99 reactions)
BENZAL	14	BALD \rightarrow nothing (see SAPRC99 reactions)
C3H7ONO2	400	i-C3H7ONO2 + hv \rightarrow i-C3H7O. + NO2
2-C5H11ONO2	900	2-C5H11ONO2 + hv \rightarrow 2-C5H11HO. + NO2
PAN	1400	PAN + hv \rightarrow CH3C(O)OO. + NO2
CH3CHO	1700	CH3CHO + hv \rightarrow CH3. + CHO.
C2H5CHO	1800	C2H5CHO + hv \rightarrow C2H5. + CHO.
n-C3H7CHO	1900	n-C3H7CHO + hv \rightarrow n-C3H7. + CHO.
n-C3H7CHO	2000	n-C3H7CHO + hv \rightarrow C2H4 + CH3CHO Norrish II
i-C3H7CHO	2100	i-C3H7CHO + hv \rightarrow C3H7. + CHO.
acetone	3000	Acetone + hv \rightarrow CH3CO + CH3
CH3COC2H5	3100	CH3COC2H5 + hv \rightarrow C2H5. + CH3CO.
CH3COC2H5	3200	CH3COC2H5 + hv \rightarrow CH3. + C2H5CO.
CH3COCH2CH(CH3)2	3600	CH3COCH2CH(CH3)2 + hv \rightarrow CH3CO. + CH2(.)
CH3COCH2CH(CH3)2	3700	CH3COCH2CH(CH3)2 + hv \rightarrow CH3COCH3 + CH2=CH(CH3) Norrish II
CH2=CHCHO	4000	CH2=CHCHO + hv \rightarrow CH2CH=CHCO. + HO2.
CH2=CHCHO	4100	CH2=CHCHO + hv \rightarrow CH2=CH. + CHO.
CH2=CHCHO	4200	CH2=CHCHO + hv \rightarrow CH3C(.)H + CO
CH2=C(CH3)CHO	4300	CH2=C(CH3)CHO + hv \rightarrow CH2=C(.)CH3 + CHO.
CH2=C(CH3)CHO	4400	CH2=C(CH3)CHO + hv \rightarrow CH3C(.)CH3 + CO
CH2=C(CH3)CHO	4500	CH2=C(CH3)CHO + hv \rightarrow CH2=C(CH3)C(.)O
CH2=CHCOCH3	4900	CH2=CHCOCH3 + hv \rightarrow CH2=CHCH3 + CO
CH2=CHCOCH3	5000	CH2=CHCOCH3 + hv \rightarrow CH2=CH. + CH3CO.
CHOCHO	5100	CHOCHO + hv \rightarrow H2 + 2CO
CHOCHO	5200	CHOCHO + hv \rightarrow 2 CHO.
CHOCHO	5300	CHOCHO + hv \rightarrow HCHO + CO
CH3COCHO	5400	CH3COCHO + hv \rightarrow CHO. + CH3CO.
CH3COCHO	5500	CH3COCHO + hv \rightarrow CO + CH3CHO
CH3COCHO	5600	CH3COCHO + hv \rightarrow 2 CO + CH4
CH3COCOCH3	5700	CH3COCOCH3 + hv \rightarrow 2 CH3CO.
OHCH2CHO	7400	OHCH2CHO + hv \rightarrow OHCH2. + .CHO
CHOCOOH	7800	CHOCOOH + hv \rightarrow CO2 + HCHO
CHOCOOH	7900	CHOCOOH + hv \rightarrow 2 CO + H2O
1-C4H9ONO2	10100	1-C5H11ONO2 + hv \rightarrow 1-C5H11HO. + NO2
2-C4H9ONO2	10200	2-C4H9ONO2 + hv \rightarrow 2-C4H9O. + NO2
aldehyde	20300	linear aldehyde (no gamma-H + Calpha primary)
RCOCHO	21400	RCOCHO + hv \rightarrow RC(.)O + CHO.
CH3COCHO	21500	CH3COCHO + hv \rightarrow CO + RCHO
CH3COCHO	21600	CH3COCHO + hv \rightarrow 2 CO + RH
n-ketone	30100	n-ketone (no gammaH) + hv \rightarrow RC(.)O + R.
n-ketone	30200	n-ketone + hv \rightarrow RC(.)O + R.
n-ketone	30300	n-ketone + hv \rightarrow Norrish II
CH2=CHCOCH3	31600	CH2=CHCOCH3 + hv \rightarrow = + CO
CH2=CHCOCH3	31700	CH2=CHCOCH3 + hv \rightarrow =. + RC(.)O
OHCH2COR	31900	OHCH2COR + hv \rightarrow RC(.)O + C(OH)(.)H2
CH3OOH	40100	CH3OOH + hv \rightarrow CH3O. + OH.

Bibliography

- R. Atkinson, D. L. Baulch, R.A. Cox, R.F. Hampson, J.A. Kerr, .M.J. Rossi, and J. Troe. Evaluated kinetics and photochemical data for atmospheric chemistry, Organic species : Supplement V. Journal of Physical Chemistry Reference Data, 26(521), 1997.
- R. Atkinson, D. L. Baulch, Cox R.A., Hampson R.F., Kerr J.A., and Rossi M.J. Evaluated kinetics and photochemical data for atmospheric chemistry, Organic species : Supplement VII. Journal of Physical Chemistry Reference Data, 28:191–392, 1999.
- W.P.L. Carter. Documentation of the SAPRC-99 chemical mechanism for VOC reactivity assessment, 2000.
- W.B. De More, S.P. Sander, D.M. Golden, R.F. Hampson, M.J. Kurylo, C.J. Howard, A.R. Ravishankara, C.E. Kolb, and M.J. Molina. Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling. Jet Propulsion Laboratory, 1997.
- S.P. Sander, R.R. Friedl, W.B. De More, D.M. Golden, R.F. Hampson, R.E. Huie, M.J. Kurylo, G.K. Moortgat, A.R. Ravishankara, C.E. Kolb, and M.J. Molina. Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling. Jet Propulsion Laboratory, 2000.
- J. Stutz, E.S. Kim, U. Platt, P. Bruno, C. Perrino, and A. Febo. UV-visible absorption cross sections of nitrous acid. Journal of Geophysical Research, 105:14585–14592, 2000.
- J. Troe. Analysis of the temperature and pressure dependance of the reaction $\text{HO} + \text{NO}_2 + \text{M} \rightleftharpoons \text{HONO}_2 + \text{M}$. International Journal of Chemical Kinetics, 33:878–879, 2001.
- G.S. Tyndall, R.A. Cox, C. Granier, R. Lesclaux, G.K. Moortgat, M.J. Pilling, A.R. Ravishankara, and T.J. Wallington. Atmospheric chemistry of small organic peroxy radicals. Journal of Geophysical Research, 106:12157–12182, 2001.