

## Appendix: The extended global chemistry mechanism

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The Appendix describes the extended photochemical mechanism used in the IMPACT model for global tropospheric photochemistry [Ito *et al.*, 2005]. The mechanism is based on the GEOS-CHEM mechanism [Evans *et al.*, 2003, version 5-07-8, available at [http://www.env.leeds.ac.uk/~mat/GEOS-CHEM/geoschem\\_mech.pdf](http://www.env.leeds.ac.uk/~mat/GEOS-CHEM/geoschem_mech.pdf)]. The extended mechanism includes all species and reactions from Evans *et al.*, 2003, except as noted or modified below.

Table A1 lists the additional species included in this mechanism. Table A2 lists the added and modified reactions.

**Table A1**

### Additional species in the extended mechanism

The extended mechanism includes all species listed in Evans *et al.* [2003].

Symbol	Formula (a sample is given for lumped species)	Description
A3N2	C <sub>3</sub> H <sub>7</sub> ONO <sub>2</sub>	Propane alkyl nitrate
A-DI	C <sub>6</sub> H <sub>5</sub> OH(OH)CHO	Product of decomposition of dicarbonyls
ACHO	C <sub>6</sub> H <sub>5</sub> CHO	Benzaldehyde
AD2P		ROOH from ADD2
ADAL	CHOCH=C(CH <sub>3</sub> )CHO	dicarbonyl
ADBP		ROOH from ADDB
ADD2	C <sub>6</sub> H <sub>5</sub> (CH <sub>3</sub> )OH(OH)O <sub>2</sub>	Secondary aromatic RO <sub>2</sub>

ADDB	$C_6H_6(OH)OO$	RO2 from benzene
ADDT	$C_6H_5(CH_3)(OH)OO$	RO2 from toluene
ADDX	$C_6H_4(CH_3)_2(OH)OO$	RO2 from m-xylene
ADTP	$C_6H_5(CH_3)(OH)OOH$	ROOH from ADDT
ADXP	$C_6H_4(CH_3)_2(OH)OOH$	ROOH from ADDX
ALK7	$C_7H_{16}$	$C_6$ - $C_8$ alkanes
AO0		radical product of AO1
AO1		radical product of AO2
AO2	$C_6H_5OH(OH)CO_3$	radical resulting from A-DI
AP	$C_6H_5OH(OH)C(O)OOH$	ROOH from AO2
APAN	$C_6H_5OH(OH)CO_3NO_2$	acyl peroxy nitrate from AO2
APIN	$C_{10}H_{16}$	$\alpha$ -pinene
ARO2	$C_6H_5CH_2O_2$	benzyl radical from toluene
ARP	$C_6H_5CH_2OOH$	ROOH from ARO2
BAP	$C_6H_5C(O)OOH$	ROOH from BCO3
BCO3	$C_6H_5CO_3$	acyl radical from benzene
BENZ	$C_6H_6$	benzene
BUO2	$HOC_4H_8O_2$	RO2 radical from <i>trans</i> -2-butene
BUP	$HOC_4H_8OOH$	ROOH from BUO2
BUTE	$C_4H_8$	<i>trans</i> -2-butene
CHO2	$CH_2O_2$	Criegee biradical
CRO2	$CH_3CHO_2$	Criegee biradical
CRES	$C_6H_4(CH_3)(OH)$	cresol
DAP	$CHOCH=CHC(O)OOH$	ROOH from DCO3
DCO1		radical product of DCO2
DCO2		radical product of DCO3
DCO3	$CHOCH=CHCO_3$	dicarbonyl acyl radical
DIAL	$CHOCH=CHCHO$	dicarbonyl
DMP	$C_6H_3OH(CH_3)_2$	dimethyl phenol
DPAN	$CHOCH=CHCO_3NO_2$	dicarbonyl PAN from DCO3
EO2	$HOC_2H_4O_2$	RO2 from ethene

EP	$\text{HOC}_2\text{H}_4\text{OOH}$	peroxide from ethene
ETHE	$\text{C}_2\text{H}_4$	ethene
IPO2		RO2 from IPRD
IPRD		misc. terpene reaction product
LIMO	$\text{C}_{10}\text{H}_{16}$	limonene
LIO2	$\text{HOC}_{10}\text{H}_{16}\text{O}_2$	RO2 from limonene
LIP	$\text{HOC}_{10}\text{H}_{16}\text{OOH}$	ROOH from limonene
MAO2		RO2 from MAO3 (methacrolein)
MDAL	$\text{CH}_3\text{COCH}=\text{CHCHO}$	dicarbonyl
NITP	$\text{C}_6\text{H}_5\text{ONO}_2$	benzyl nitrate
PBZN	$\text{C}_6\text{H}_5\text{CO}_3\text{NO}_2$	acyl peroxy nitrate from benzene (BCO3)
PHEN	$\text{C}_6\text{H}_5\text{OH}$	phenol
PHO2	$\text{C}_6\text{H}_5\text{O}_2$	secondary RO2 from benzene
PHP	$\text{C}_6\text{H}_5\text{OOH}$	ROOH from PHO2
PIN2	$\text{ONO}_2\text{C}_{10}\text{H}_{16}\text{O}_2$	RO2 from terpenes+NO3
PINT	$\text{ONO}_2\text{C}_{10}\text{H}_{16}\text{OOH}$	ROOH from terpenes+NO3
PIO2	$\text{HOC}_{10}\text{H}_{16}\text{O}_2$	RO2 from $\alpha$ -pinene
PIP	$\text{HOC}_{10}\text{H}_{16}\text{OOH}$	ROOH from from $\alpha$ -pinene
POXY	$\text{C}_6\text{H}_5\text{O}$	aromatic radical
R3N1		RO2 from propane alkyl nitrate
R5N1		RO2 from R6N1
R6N1		RO2 from R7N1
R7N1		RO2 from C <sub>6</sub> -C <sub>8</sub> alkyl nitrates
R7O2	$\text{C}_7\text{H}_{15}\text{O}_2$	RO2 from C <sub>6</sub> -C <sub>8</sub> alkanes
R7O1		Secondary RO2 from R7O2
R7P	$\text{C}_7\text{H}_{15}\text{OOH}$	ROOH from C <sub>6</sub> -C <sub>8</sub> alkanes
TOLU	$\text{C}_6\text{H}_5(\text{CH}_3)$	toluene (representing alkylbenzenes)
XAP	$\text{CH}_3\text{COCH}=\text{CH}(\text{O})\text{OOH}$	ROOH from XCO3 (dicarbonyl)
XCO1		radical product of XCO2

XCO2		radical product of XCO3
XCO3	$\text{CH}_3\text{COCH}=\text{CHCO}_3$	dicarbonyl acyl radical
XPAN	$\text{CH}_3\text{COCH}=\text{CHCO}_3\text{NO}_2$	dicarbonyl PAN from XCO3
XYLE	$\text{C}_6\text{H}_4(\text{CH}_3)_2$	m-xylene (representing dialkylbenzenes)
YAP	$\text{CHOCH}=\text{C}(\text{CH}_3)\text{C}(\text{O})\text{OOH}$	ROOH from YCO3 (dicarbonyl)
YCO1		radical product of YCO2
YCO2		radical product of YCO3
YCO3	$\text{CHOCH}=\text{C}(\text{CH}_3)\text{CO}_3$	dicarbonyl acyl radical
YPAN	$\text{CHOCH}=\text{C}(\text{CH}_3)\text{CO}_3\text{NO}_2$	dicarbonyl PAN from YCO3
ZAP	$\text{CHOC}(\text{CH}_3)=\text{CHC}(\text{O})\text{OOH}$	ROOH from ZCO3 (dicarbonyl)
ZCO1		radical product of ZCO2
ZCO2		radical product of ZCO3
ZCO3	$\text{CHOC}(\text{CH}_3)=\text{CHCO}_3$	dicarbonyl acyl radical
ZPAN	$\text{CHOC}(\text{CH}_3)=\text{CHCO}_3\text{NO}_2$	dicarbonyl PAN from ZCO3

**Table A2****Additional and modified reactions in the extended mechanism**

The extended mechanism includes all reactions listed in *Evans et al.* [2003], except for the reactions replaced by modified forms in the table.

Abbreviations: HPL= High Pressure Limit. LPL=Low Pressure Limit. T=Temperature.

Units are molec cm<sup>-3</sup>s<sup>-1</sup> for reactions involving two species and s<sup>-1</sup> for reactants involving a single species.

Reaction	Rate constant	References	Notes
<i>Isoprene and products</i>			
RIO2 + NO => 1.0 ISN2	K*Yn where Yn is the nitrate yield based on carbon number (=5.). K=2.7E-12 exp(350/T)	IUPAC, 2003; Sprengnether, 2002	modified reaction; same rate as <i>Evans</i> , 2003.
RIO1 + NO => 1.0 ISN2	K*Yn where Yn is the nitrate yield based on carbon number (=5.). K=2.7E-12 exp(350/T)	IUPAC, 2003; Sprengnether, 2002	modified reaction; same rate as <i>Evans</i> , 2003.
VRO2 + NO =>1.0 ISN2	K*Yn where Yn is the nitrate yield based on carbon number (=4.). K=2.7E-12 exp(350/T)	IUPAC,2003	modified reaction; same rate as <i>Evans</i> , 2003.
MRO2 + NO =>1.0 ISN2	K*Yn where Yn is the nitrate yield based on carbon number (=4.). K=2.700E-12 exp(350/T)	IUPAC, 2003	modified reaction; same rate as <i>Evans</i> , 2003.

INO2 +NO => 0.05 MVK + 0.1 MACR + 0.15 HCHO+ 0.85 ISN2 + 1.15 NO2 + 0.8 HO2	2.7E-12 exp(350/T)	Tyndall, 2001 ETO2+NO	same rate as <i>Evans et al.</i> , 2003, ISN2 replaces HNO3
ISN2 + OH => 1.0 ISN1	3.210e-11	Paulson and Seinfeld, 1992; Treves and Rudich, 2003	added reaction
RIP + OH => 0.5 IAO2 + 0.4 RIO2 + 0.2 RIO1	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	Rate based on MACR+OH rather than MP+OH
IAP + OH => 0.5 OH + 0.18 HAC + 0.5 IAO2 + 0.335 CO + 0.13 GLYC + 0.29 MGLY	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	RCHO product replaced by equiv. products of IAO2+NO
ISNP + OH => 0.5 OH + 0.5 MGLY + 0.5 ISN1 + 0.5 NO2	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	RCHO product replaced by equiv. products of ISN1+NO
VRP + OH => 0.5 OH + 0.5MGLY + 0.5 VRO2 + 0.14 HCHO + 0.36 GLYC	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	RCHO product replaced by equiv. products of VRO2+NO

MRP + OH => 0.5 OH + 0.415 HAC + 0.5 MRO2 + 0.085 MGLY + 0.415 CO + 0.085 HCHO	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	RCHO product replaced by equiv. products of MRO2+NO
MAOP + OH => 0.5 OH + 1.0 HCHO + 0.5 MAO3	8.0E-12 exp(380/T)	Paulson and Seinfeld, 1992; IUPAC 2003 rate for MACR	RCHO product replaced by equiv. products of IAO2+NO
<b><i>Terpenes and products</i></b>			
APIN + OH => 1.0 PIO2	1.210E-11 exp(444/T)	Stockwell, 1997	
PIO2 + NO => 0.8 ALD2 + 0.8MEK + 0.2 PINT + 0.8 HO2 + 0.8 NO2	4.901E-12 exp(180/T)	Stockwell, 1997	
PIO2 + HO2 => 1.0 PIP	7.4E-13 exp(700/T)	Stockwell, 1997, Tyndall, 2001	
APIN + O3 => 0.065 ALD2 + 0.53 MEK + 0.14 CO + 0.2 EO2 + 0.42 KO2 + 0.85 OH + 0.1 HO2 + 0.02 H2O2	1.010E-15 exp(-732/T)	Stockwell, 1997	
APIN + NO3 => 0.1 INO2 + 0.9 PIN2	1.190E-12 exp(490/T)	Stockwell, 1997	

PIN2 + NO => 0.287 HCHO + 1.24 ALD2 + 0.464 MEK + 2.000 NO2	4.901E-12 -180.	Stockwell, 1997	
PIN2 + HO2 => 1.0 ISNP	3.0E-12	Stockwell, 1997	
PINT + OH => 1.0 ISNR	3.210E-11	Treves and Rudich, 2003	Equivalent to hydroxyalkyl nitrate from isoprene
LIMO + OH => 1.0 LIO2	1.710E-10	Stockwell, 1997	
LIO2 + NO => 0.4 IPRD + 0.25BUTE + 0.25 HCHO + 0.65 HO2 + 0.65 NO2 + 0.35 PINT	4.901E-12 exp(180/T)	Stockwell, 1997	lumped products changed to equivalents
LIO2 + HO2 => 1.0 LIP	7.4E-13 exp(700/T)	Stockwell, 1997, Tyndall, 2001	
LIMO+O3 => 0.04 HCHO + 0.46 PRPE + 0.14 CO + 0.16 EO2 + 0.42 KO2 + 0.85 OH + 0.1 HO2 + 0.02 H2O2 + 0.79 MACR + 0.08 HCOOH	2.000E-16	Stockwell, 1997	
LIMO + NO3 => 0.13 INO2 + 0.87 PIN2	1.220E-11	Stockwell, 1997	
IPRD + OH => 1.0 IPO2	6.190E-11	Carter, 1996	



IPO2 + NO => 0.418 CO + 1.0 NO2 + 0.687 HO2 + 0.125 GLYC + 0.124 GLYX + 0.062 RCHO +0.145 MGLY + 0.48 HAC + 0.313 MAO3	4.901E-12 exp(180/T)	Carter, 1996	
IPO2 + HO2 => 1.0 MRP	7.4E-13 exp(700/T)	Carter, 1996, Tyndall, 2001	
PIP + OH => 0.5PIO2 + 1.0 HO2 + 0.5 ALD2 + 0.5 MEK	3.8E-12 exp(200/T)	Stockwell, 1997; JPL 2003	
PIP + O3 => 0.7 HCHO	8.0E-21	Stockwell,1997	
LIP + OH => 0.5 LIO2 + 1.0 HO2 + 0.3 IPRD + 0.19 BUTE + 0.19 HCHO	3.8E-12 exp(200/T)	Stockwell, 1997; JPL 2003	MACR replaced by IPRD (MACR is exact spec.)
LIP + O3 => 0.7 HCHO	8.0E-21	Stockwell,1997	
PIP + hv => 1.0 HAC + 1.0 OH + 1.0 HO2	5.0E-04 j <sub>NO2</sub>	Stockwell, 1997	
LIP + hv => 1.0 HAC + 1.0 OH + 1.0 HO2	5.0E-04 j <sub>NO2</sub>	Stockwell, 1997	
<b><i>Alkanes and alkenes</i></b>			
ALK7 + OH => 1.0 R7O2	2.000E-11 exp(- 359/T)	Lurmann et al., 1986	
R7O2 + NO => 0.75 R7O1 + 0.25 R4O2 + 0.25 MEK + 1.0 NO2	K*(1-Y <sub>n</sub> ) where Y <sub>n</sub> is the nitrate yield based on carbon number (=7). K=4.901E-12 exp(180/T)	Lurmann et al., 1986	

R7O2 + NO => 1.0 R7N2	K*Yn where Yn is the nitrate yield based on carbon number (=7.). K=4.901E-12 exp(180/T)	Lurmann et al., 1986	
R7O1 + NO => 1.0 RCHO + 1.0 NO2 + 1.0 HO2	K*(1-Yn) where Yn is the nitrate yield based on carbon number (=7.). K=4.901E-12 exp(180/T)	Lurmann et al., 1986	
R7O1 + NO => 1.0 R7N2	K*Yn where Yn is the nitrate yield based on carbon number (=7.). K=4.901E-12 exp(180/T)	Lurmann et al., 1986	
ALK7 + NO3 => 1.0 R7O2 + 1.0 HNO3	6.000E-17	Lurmann et al., 1986	
R7N2 + OH => 1.0 R7N1	4.901E-12 exp(180/T)	Lurmann et al., 1986	
R7N1 + NO => 0.11 R6N1 + 0.65 R5N1 + 0.65 ALD2 + 0.11 HCHO +0.48 RCHO + 1.24 NO2	4.901E-12 exp(180/T)	Lurmann et al., 1986	
R6N1 + NO => 1.0 R5N1 + 1.0 HCHO + 1.0 NO2	4.901E-12 exp(180/T)	Lurmann et al., 1986	
R5N1 + NO => 1.0 HCHO + 1.0 RCHO + 2.0 NO2	4.901E-12 exp(180/T)	Lurmann et al., 1986	

R7O2 + HO2 => 1.0 R7P	7.4E-13 exp(700/T)	Tyndall, 2001	
R7N1 + HO2 => 1.0 R7N2	7.4E-13 exp(700/T)	Tyndall, 2001	
R6N1 + HO2 => 1.0 R7N2	7.4E-13 exp(700/T)	Tyndall, 2001	
R5N1+HO2 => 1.0 R4N2	7.4E-13 exp(700/T)	Tyndall, 2001	
ETHE + OH => 1.0 EO2	LPL: 7E-29(T/300) <sup>-3.1</sup> HPL:9E-12	IUPAC, 2003	
EO2 + NO => 1.6 HCHO + 0.20 GLYC + 1.0 NO2 + 1.0 HO2	9.000E-12	Lurmann et al., 1986	
EO2 + HO2 => 1.0 EP	7.4E-13 exp(700/T)	Tyndall, 2001	
ETHE + O3 => 1.0 HCHO + 0.4 CHO2 + 0.2 HO2 + 0.06 CH4 + 0.42 CO + 0.2 OH	9.500E-15 exp(-2580/T)	IUPAC, 2003	
BUTE + OH => 1.0 BUO2	1.100e-11 exp(549/T)	Lurmann, 1986	
BUO2 + NO => 1.8 ALD2 + 0.1 R4N2 + 0.9 NO2 + 0.9 HO2	4.901E-12 exp(180/T)	Lurmann et al., 1986	
BUO2 + HO2 => 1.0 BUP	7.4E-13 exp(700/T)	Tyndall, 2001	
BUTE + O3 => 1.0 ALD2 + 0.4 CRO2 + 0.25 HO2 + 0.6 OH + 0.35 MO2	7.5E-15 exp(-1050/T)	Lurmann et al., 1986	

CHO2 + NO => 1.0 HCHO + 1.0 NO2	7.0e-12	Lurmann, 1986	
CHO2 + NO2 => 1.0 HCHO + 1.0 NO3	7.0e-13	Lurmann, 1986	
CHO2+H2O =>1.0 HCOOH	4.0E-18	Lurmann, 1986	
CRO2 + NO => 1.0 ALD2 + 1.0NO2	7.0e-12	Lurmann, 1986	
CRO2 + NO2 => 1.0 ALD2 + 1.0 NO3	7.0e-13	Lurmann, 1986	
CRO2+H2O =>1.0 HCOOH	4.0E-18	Lurmann, 1986	
SO2 + CHO2 => 1.0 HCHO + 1.0 HSO4	7.0E-14	Lurmann, 1986	
SO2 + CRO2 => 1.0 ALD2 + 1.0 HSO4	7.0E-14	Lurmann, 1986	
CHO2 + HCHO => products	1.360e-14	Lurmann, 1986	
CHO2 + ALD2 => products	1.360e-14	Lurmann, 1986	
CRO2 + HCHO => products	1.360e-14	Lurmann, 1986	
CRO2 + ALD2 => products	1.360e-14	Lurmann, 1986	
R7P + OH => 0.5 R7O2 + 0.5RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
EP + OH => 0.5 EO2 + 0.5 GLYC + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
BUP + OH => 0.5BUO2 + 0.5 RCHO + 1.0 HO2	3.8E-12 exp(200/T)	JPL 2003	

R7P + hv => 1.0 RCHO + 1.0 OH + 1.0 HO2	5.0E-04 j <sub>NO2</sub>	Lurmann, 1986	
EP + hv => 1.0 GLYC + 1.0 OH + 1.0 HO2	5.0E-04 j <sub>NO2</sub>	Lurmann, 1986	
BUP + hv => 1.0 RCHO + 1.0 OH + 1.0 HO2	5.0E-04 j <sub>NO2</sub>	Lurmann, 1986	
<i>Aromatics</i>			
BENZ + OH => 0.25 PHEN + 0.75 ADDB + 0.25 HO2	2.330E-12 exp(-193/T)	Lurmann, 1986; Atkinson and Arey, 2003	
ADDB + NO => 1.0 DIAL + 1.0 GLYX + 1.0 NO2 + 1.0 HO2	4.901E-12 exp(180/T)	Lurmann, 1986	
TOLU + OH => 0.16 CRES + 0.08 ARO2 + 0.76 ADDT + 0.16 HO2	1.180E-12 exp(338/T)	Lurmann, 1986	
ARO2 + NO => 0.9 ACHO + 0.1 R4N2 + 0.9 NO2 + 0.9 HO2	4.901E-12 exp(180/T)	Lurmann, 1986	
ADDT + NO => 0.8 MGLY + 0.8 DIAL + 0.2 GLYX + 0.05 MDAL + 0.15 ADAL + 1.0 NO2 + 1.0 HO2	4.901E-12 exp(180/T)	Lurmann, 1986	

XYLE + OH =>0.83 ADDX + 0.17 DMP + 0.17 HO2	2.400e-11	Lurmann, 1986	
ADDX + NO => 1.0 MGLY + 0.5 MDAL + 0.5 ADAL + 1.0 NO2 + 1.0 HO2	4.901E-12 exp(180/T)	Lurmann,1986	
PHEN + OH => 0.9 ADD2 + 0.1 POXY	2.800E-11	Lurmann, 1986	
CRES + OH => 0.9 ADD2 + 0.1 POXY	4.250E-11	Lurmann, 1986	
DMP + OH => 0.9 ADD2 + 0.1 POXY	7.000E-11	Lurmann, 1986	
POXY + NO2 => 1.0NITP	1.500E-11	Lurmann, 1986	
ADD2 + NO => 1.0 A- DI + 1.0NO2 + 1.0 HO2	4.901E-12 exp(180/T)	Lurmann, 1986	
A-DI + OH => 1.0 AO2	1.500e-11	Lurmann, 1986	
AO2 + NO2 => 1.0 APAN	4.700e-12	Lurmann, 1986	
APAN => 1.0 AO2 + 1.0 NO2	1.950E+16 exp(-13543/T)	Lurmann, 1986	
AO2 + NO => 1.0 AO1 + 1.0 NO2	2.0E-11	Lurmann, 1986	
AO1 + NO => 1.0 AO0 + 1.0 NO2	2.0E-11	Lurmann, 1986	
AO0 + NO => 1.0GLYX + 1.0 CO + 1.0 NO2 + 1.0 HO2	2.0E-11	Lurmann, 1986	

PHEN + NO3 => 1.0 POXY + 1.0 HNO3	2.0E-12	Lurmann, 1986	
CRES + NO3 => 1.0 POXY + 1.0 HNO3	1.0E-11	Lurmann, 1986	
DMP + NO3 => 1.0 POXY + 1.0 HNO3	1.5E-11	Lurmann, 1986	
NITP + NO3 => 1.0 R4N2 + 1.0 HNO3	1.0E-11	Lurmann, 1986	modified to conserve reactive nitrogen
DIAL + OH => 1.0 DCO3	3.0E-11	Lurmann, 1986	
MDAL+ OH => 1.0 XCO3	1.5E-11	Lurmann, 1986	
ADAL+ OH => 0.5 YCO3 + 0.5 ZCO3	3.0E-11	Lurmann, 1986	
DCO3+ NO2 => 1.0 DPAN	4.700E-12	Lurmann, 1986	
XCO3+ NO2 => 1.0 DPAN	4.700E-12	Lurmann, 1986	
YCO3+ NO2 => 1.0 DPAN	4.700E-12	Lurmann, 1986	
ZCO3+ NO2 => 1.0 DPAN	4.700E-12	Lurmann, 1986	
DPAN => 1.0 DCO3 + 1.0 NO2	1.950E+16 exp(-13543/T)	Lurmann, 1986	
XPAN => 1.0 XCO3 + 1.0 NO2	1.950E+16 exp(-13543/T)	Lurmann, 1986	
YPAN => 1.0 YCO3 + 1.0 NO2	1.950E+16 exp(-13543/T)	Lurmann, 1986	

ZPAN => 1.0 ZCO3 + 1.0 NO2	1.950E+16 exp(-13543/T)	Lurmann, 1986	
DCO3 + NO => 1.0 DCO2 + 1.0 NO2	2.0E-11	Lurmann, 1986	
DCO2 + NO => 1.0 DCO1 + 1.0 NO2	2.0E-11	Lurmann, 1986	
DCO1 + NO => 1.0 GLYX + 1.0 CO + 1.0 NO2 + 1.0 HO2	2.0E-11	Lurmann, 1986	
XCO3 + NO => 1.0 XCO2 + 1.0 NO2	2.0E-11	Lurmann, 1986	
XCO2 + NO => 1.0 XCO1 + 1.0 NO2	2.0E-11	Lurmann, 1986	
XCO1 + NO => 0.5 MGLY + 0.5 MCO3 + 0.5 GLYX + 1.000 CO + 1.000 NO2 + 0.500 HO2 + 1.0 CO + 1.0 NO2 + 0.5 HO2	2.0E-11	Lurmann, 1986	
YCO3 + NO => 1.0 YCO2 + 1.0 NO2	2.0E-11	Lurmann, 1986	
YCO2 + NO => 1.0 YCO1 + 1.0 NO2	2.0E-11	Lurmann, 1986	
YCO1 + NO => 0.5 MGLY + 0.5 MCO3 + 0.5 GLYX + 2.0 CO + 1.0 NO2 + 0.5 HO2 + 1.0 NO2 + 0.5 HO2	2.0E-11	Lurmann, 1986	



ZCO3 + NO => 1.0 ZCO2 + 1.0 NO2	2.0E-11	Lurmann, 1986	
ZCO2 + NO => 1.0 ZCO1 + 1.0 NO2	2.0E-11	Lurmann, 1986	
ZCO1 + NO => 1.0 MGLY + 1.0 CO + 1.0 NO2 + 1.0 HO2	2.0E-11	Lurmann, 1986	
DIAL + hv => 1.0 DCO3 + 1.0 HO2	5.0E-03 j <sub>NO2</sub>	Lurmann, 1986	
MDAL +hv =>0.5 DCO3 +0.5 XCO3 + 0.5 MCO3 + 0.5 HO2	3.0E-02 j <sub>NO2</sub>	Lurmann, 1986	
ADAL + hv =>0.5 YCO3 + 0.5 ZCO3 + 1.0 HO2	3.0E-02 j <sub>NO2</sub>	Lurmann, 1986	
ACHO+OH => 1.0BCO3	1.2E-11	Lurmann, 1986	
BCO3+NO2=>1.0 PBZN	4.7E-12	Lurmann, 1986	
PBZN => 1.0 BCO3 + 1.0 NO2	1.95E+16exp(-13543/T)	Lurmann, 1986	
BCO3 + NO =>1.0 PHO2 + 1.0 NO2	2.0E-11	Lurmann, 1986	
PHO2 +NO =>1.0 POXY + 1.0NO2	2.0E-11	Lurmann, 1986	
ADDB+HO2=>1.0 ADBP	7.4E-13 exp(700/T)	Tyndall, 2001	
ARO2 +HO2 => 1.0ARP	7.4E-13 exp(700/T)	Tyndall, 2001	
ADDT+HO2=>1.0 ADTP	7.4E-13 exp(700/T)	Tyndall, 2001	
ADDX+HO2=>1.0ADXP	7.4E-13 exp(700/T)	Tyndall, 2001	
ADD2+HO2=>1.0 AD2P	7.4E-13 exp(700/T)	Tyndall, 2001	
AO2 + HO2 => 0.75 AP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	Plus identical reaction for AO1, AO0

DCO3+ HO2=>0.75 DAP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	Plus identical reaction for DCO2, DCO1
XCO3+ HO2=>0.75 XAP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	Plus identical reaction for XCO2, XCO1
YCO3+ HO2=>0.75 YAP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	Plus identical reaction for YCO2, YCO1
ZCO3+ HO2=>0.75 ZAP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	Plus identical reaction for ZCO2, ZCO1
PHO2+ HO2=>0.75 PHP + 0.25 EOH + 0.25 O3	7.4E-13 exp(700/T)	Tyndall, 2001	
ADBP+OH =>1.0 ADDB	3.8E-12 exp(200/T)	JPL 2003	
ARP+OH =>1.0 ARO2	3.8E-12 exp(200/T)	JPL 2003	
ADTP+OH =>1.0 ADDT	3.8E-12 exp(200/T)	JPL 2003	
ADXP+OH=>1.0 ADDX	3.8E-12 exp(200/T)	JPL 2003	
AD2P+OH =>1.0 ADD2	3.8E-12 exp(200/T)	JPL 2003	
BAP+OH =>1.0 BCO3	3.8E-12 exp(200/T)	JPL 2003	
PHP+OH =>1.0 PHO2	3.8E-12 exp(200/T)	JPL 2003	
AP+OH => 0.5 AO2 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
AP+OH => 0.5 AO2 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
DAP+OH => 0.5 DCO3 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
XAP+OH => 0.5 XCO3 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
YAP+OH => 0.5 YCO3 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	

ZAP+OH => 0.5 ZCO3 + 0.5 RCHO + 0.5 OH	3.8E-12 exp(200/T)	JPL 2003	
ADTP +hv=> 1.0 RCHO + 1.0 OH + 1.0 HO2	1.0E-03 j <sub>NO2</sub>	Lurmann, 1986	Plus identical reaction for ADXP, AD2P, BAP and PHP
APAN, DPAN + OH =>1.0 GLYX + 1.0 NO2	4.0E-14	JPL, 2003	Identical reaction for APAN, DPAN
XPAN+OH =>0.5 MGLY + 0.5 GLYX + 1.0 NO2	4.0E-14	JPL, 2003	
YPAN, ZPAN + OH => 1.00 MGLY + 1.0 NO2	4.0E-14	JPL, 2003	Identical reaction for YPAN, ZPAN
PBZN + OH =>1.0 POXY + 1.0 NO2	4.0E-14	JPL, 2003	
IPAN + OH =>1.0 HCHO + 1.0 NO2	4.0E-14	JPL, 2003	
<b>Additional RO2-RO2 reactions</b>			
MO2+R7O2=> 1.0 HCHO + 1.0 HO2 +0.35 RCHO+ 0.07 ALD2 + 0.14 ACET + 0.28 MEK	8.37E-14	Tyndall, 2001 MO2+MO2, Atkinson, 1997 RO2+RO2	see note in Evans et al., 2003
MO2+EO2=> 1.0 HCHO + 1.0 HO2 +0.55 HCHO+0.45 ALD2	5.92E-13	Tyndall, 2001 MO2+MO2, Atkinson, 1997 RO2+RO2	see note in Evans et al., 2003

MO2+BUO2=> 1.0 HCHO + 1.0 HO2 +0.19 MEK+0.93 ALD2	5.92E-13	Tyndall, 2001 MO2+MO2, Atkinson, 1997 RO2+RO2	see note in <i>Evans et al.</i> , 2003
MO2+ADDT=> 1.0 HCHO + 1.0 HO2 +0.16GLYX+ 0.17MGLY +0.92 HO2+ 0.05 MCO3 +0.56 DIAL+0.035MDAL + 0.105 ADAL	3.56E-14 exp(708/T)	Stockwell, 1997	
MO2+ADDX=> 1.0 HCHO + 1.0 HO2 +0.45 MGLY+0.4 MDAL +1.0 HO2 +0.406 ADAL	3.56E-14 exp(708/T)	Stockwell, 1997	
MO2+PIO2=> 1.0 HCHO + 1.0 HO2 +1.0 ALD2 + 1.0 MEK + 1.0 HO2	3.56E-14 exp(708/T)	Stockwell, 1997	
MO2+LIO2=> 1.0 HCHO + 1.0 HO2 +0.6 IPRD + 0.38 BUTE + 0.38 HCHO + 1.0 HO2	3.56E-14 exp(708/T)	Stockwell, 1997	
MCO3 + R7O2 => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0.1 ALD2 + 0.4 RCHO +0.19 ACET + 0.39 MEK	1.85E-12 exp(500/T)	Stockwell, 1997; Tyndall MCO3+MO2, as in <i>Evans</i> , 2003	

MCO3 + EO2 => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0. HCHO + 0.6 ALD2	1.85E-12 exp(500/T)	Stockwell, 1997; Tyndall MCO3+MO2, as in <i>Evans et al.</i> , 2003	
MCO3 + BUO2 => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0.569MEK+0.941 ALD2	1.85E-12 exp(500/T)	Stockwell, 1997; Tyndall MCO3+MO2, as in <i>Evans et al.</i> , 2003	
MCO3 + ADDT => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0.65 GLYX+0.35MGLY + 0.05 MDAL +0.15ADAL + 0.8 DIAL	1.85E-12 exp(500/T)	Lurmann, 1986; Tyndall, 2001 MCO3+MO2, as in <i>Evans et al.</i> , 2003	
MCO3 + ADDX => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0.37GLYX+0.63 MGLY +0.5 MDAL + 0.5 ADAL	1.85E-12 exp(500/T)	Lurmann, 1986; Tyndall, 2001 MCO3+MO2, as in <i>Evans et al.</i> , 2003	
MCO3 + PIO2 => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +1.0 ALD2 + 1.0 MEK	1.85E-12 exp(500/T)	Stockwell, 1997; Tyndall, 2001 MCO3+MO2, as in <i>Evans et al.</i> , 2003	

MCO3 + LIO2 => 0.5 HCOOH + 0.5 HO2 + 0.5 MO2 +0.6 IPRD + 0.4 BUTE + 0.4 HCHO	1.85E-12 exp(500/T)	Stockwell, 1997; Tyndall, 2001 MCO3+MO2, as in <i>Evans et al.</i> , 2003	
RIO2 + RIO2 => 0.68 MVK + 0.39 MACR + 0.93 IPRD + 1.07HCHO + 1.38 HO2	4.2E-13	Paulson, 1992	
IPO2 + IPO2 => 0.82CO +1.374HO2+0.626 MAO3 + 0.250 GLYC+ 0.248 GLYX + 0.124 RCHO + 0.29 MGLY + 0.96 HAC	4.2E-13	Stockwell, 1997	
VRO2 + VRO2 => 1.4 HO2 + 2.0 MGLY + 1.4 HCHO	1.4E-12	Paulson, 1992	
MRO2 + MRO2 => 1.4 HO2 + 2.0 MGLY + 1.4 HCHO	1.4E-12	Paulson, 1992	
RIO2+IPO2, VRO2, MRO2=> products	average of two RO2- RO2 self-reactions		products equivalent to RO2-RO2 self-reactions
EO2 + EO2 =>1.2 GLYC + 1.2 HO2 + 0.4 EOH+ 0.4 ALD2	1.0E-12	Lurmann, 1986	

PO2 + PO2 => 1.2 RCHO + 1.2 HO2 + 0.4 EOH + 0.4 ALD2	1.0E-12	Lurmann, 1986	
KO2 + KO2 => 2.0 ALD2 + 0.44 ACET	1.0E-12	Lurmann, 1986	
RCO3 + RCO3 => 2.0 ETO2	2.5E-12 exp(500/T)	Tyndall, 2001 MCO3 rate	
MAO3 + MAO3 => 2.0 MAO2	2.5E-12 exp(500/T)	Tyndall, 2001 MCO3 rate	
MO2 + MAO3 => 0.85 MAO2 + 0.15 EOH + 1.0 HCHO	1.85E-12 exp(500/T)	Tyndall, 2001 MCO3 + MO2, as in <i>Evans et al.</i> , 2003	
MCO3 + MAO3 => 1.0 MAO2 + 1.0 MO2	2.5E-12 exp(500/T)	Tyndall, 2001 MCO3 rate	
DCO3 + DCO3 => 2.0 DCO1	2.5E-12 exp(500/T)	Tyndall, 2001 MCO3 rate	Plus equivalent reactions for AO2, XCO3, YCO3, ZCO3, BCO3
MO2 + DCO3 => 0.85 DCO1 + 0.15 EOH + 1.0 HCHO	1.85E-12 exp(500/T)	Tyndall, 2001, as in <i>Evans et al.</i> , 2003	Plus equivalent reactions of MO2 with AO2, XCO3, YCO3, ZCO3, BCO3

MCO3 + DCO3 => 1.0 DCO1 + 1.0 MO2	2.5E-12 exp(500/T)	Tyndall, 2001 MCO3 rate	Plus equivalent reactions of MCO3 with AO2, XCO3, YCO3, ZCO3, BCO3
<b>Other added reactions</b>			
RCOOH + OH => 1.0 ETO2 + 1.0 CO2	4.0E-13 exp(200/T)	JPL 2003	added by analogy to ACTA+OH
PAN + OH => 1.0 HCHO + 1.0 NO2	4.0E-14	JPL, 2003	
PPN + OH => 1.0 ALD2 + 1.0 NO2	7.5E-12 exp(-651/T)	Kasting, 1986	
DMS + OH => 1.0 SO2 + 1.0 MO2 + 1.0 HCHO	1.2E-11 exp(-260/T)	JPL 2003	
DMS + NO3 => 1.0 SO2 + 1.0 MO2 + 1.0 HCHO + 1.0 HNO3	1.9E-13 exp(500/T)	JPL 2003	
SO2 + OH => 1.0 HSO4 + 1.0 HO2	LPL: 3E-31(T/300) <sup>-3.3</sup> HPL:1.5E-12	JPL 2003	

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