

*Geophysical Research Letters*

Supporting Information for

**The Global Reactive Organic Carbon Budget: A Modeling Perspective**

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**Table 1.** Standard gas-phase mechanism species. Added and improved deposition properties are marked in bold and italic respectively. All added peroxides deposition is treated like methylhydroperoxide (CH3OOH)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| GEOS-Chem Species | Formula (in some cases illustrative) | Description | Molar Mass | | K\*298  [M/atm] | -H298/R  [k] |
| [g/mol] | [#C] |
| A3O2 | CH3CH2CH2OO | Primary RO2 from C3H8 | 75 | 3 |  |  |
| ACET | CH3C(O)CH3 | Acetone | 58 | 3 | **27.4** | **5500** |
| ACTA | CH3C(O)OH | Acetic acid | 60 | 2 | **4.05 x103** | **6200** |
| ALD2 | CH3CHO | Acetaldehyde | 44 | 2 | **13.2** | **5900** |
| ALK4 | C4H10 | >=C4 alkanes | 58 | 4 | **1.22 x10-3** | **3100** |
| ASOA11 |  | Lumped semivolatile aerosol products of light aromatics and IVOCs | 150 | 11 | As aerosol |  |
| ASOA2 |  | Lumped semivolatile aerosol products of light aromatics and IVOCs | 150 | 11 | As aerosol |  |
| ASOA3 |  | Lumped semivolatile aerosol products of light aromatics and IVOCs | 150 | 11 | As aerosol |  |
| ASOAN |  | Lumped nonvolatile aerosol products of light aromatics and IVOCs | 150 | 11 | As aerosol |  |
| ASOG12 |  | Lumped semivolatile gas products of light aromatics and IVOCs | 150 | 11 | 1.0x105 | 6039 |
| ASOG2 |  | Lumped semivolatile gas products of light aromatics and IVOCs | 150 | 11 | 1.0x105 | 6039 |
| ASOG3 |  | Lumped semivolatile gas products of light aromatics and IVOCs | 150 | 11 | 1.0 x105 | 6039 |
| ATO2 | CH3C(O)CH2O2 | RO2 from acetone | 89 | 3 |  |  |
| ATOOH | CH3C(O)CH2OOH | ATO2 peroxide | 90 | 3 |  |  |
| B3O2 | CH3CH(OO)CH3 | Secondary RO2 from C3H8 | 75 | 3 |  |  |
| C2H6 | C2H6 | Ethane | 30 | 2 | **1.93 x10-3** | **2400** |
| C3H8 | C3H8 | Propane | 44 | 3 | **1.52 x10-3** | **2700** |
| CH4 | CH4 | Methane | 16 | 1 |  |  |
| CO | CO | Carbon monoxide | 28 | 1 |  |  |
| CO2 | CO2 | Carbon dioxide | 44 | 1 |  |  |
| CH2Br2 | CH2Br2 | Dibromomethane | 174 | 1 | **1.22** | **5000** |
| CH2O | CH2O | Formaldehyde | 30 | 1 | *3.24**x103* | *6800* |
| CH3Br | CH3Br | Methyl bromide | 95 | 1 | **1.32 x10-1** | **2800** |
| CHBr3 | CHBr3 | Bromoform | 253 | 1 | **1.72** | **5200** |
| DHMOB | HOCH2C(CH3)(OH)C(=O)CHO | Multi hydroxy ketone/aldehyde from isoprene chemistry | 132 | 5 | **7.80 x103** | **0** |
| DIBOO | C5H9O5 | peroxy radical from RIO2 | 148 | 5 |  |  |
| DMS | (CH3)2S | Dimethylsulfide | 62 | 2 | **47.6** | **3100** |
| EOH | C2H5OH | Ethanol | 46 | 2 | **1.93 x102** | **6400** |
| ETHLN | CHOCH2ONO2 | Ethanal nitrate | 105 | 2 | **1.70 x104** | **9200** |
| ETO2 | CH3CH2OO | Ethylperoxy radical | 61 | 2 |  |  |
| ETP | CH3CH2OOH | Ethylhydroperoxide | 62 | 2 | **3.34 x102** | **6000** |
| GLYC | HOCH2CHO | Glycoaldehyde (hydroxyacetaldehyde) | 60 | 2 | 4.15x104 | 4600 |
| GLYX | CHOCHO | Glyoxal | 58 | 2 | *4.15* x*105* | *7500* |
| H | H | Hydrogen atom | 1 |  |  |  |
| H2 | H2 | Hydrogen molecule | 2 |  |  |  |
| H2O | H2O | Water vapor | 18 |  |  |  |
| H2O2 | H2O2 | Hydrogen peroxide | 34 |  | 8.3x104 | 7400 |
| HAC | HOCH2C(O)CH3 | Hydroxyacetone | 74 | 3 | **7.80 x103** | **0** |
| HC5 | HOCH2CH=C(CH3)CHO | Hydroxycarbonyl with 5C | 100 | 5 | **7.80 x103** | **0** |
| HC5OO | HOCH2C(CH3)(OO)CH(OH)CHO | RO2 from HC5 oxidation product | 149 | 5 |  |  |
| HCOOH | HCOOH | Formic acid | 46 | 1 | **8.92 x103** | **6100** |
| HNO2 | HNO2 | Nitrous acid | 47 |  | **47** | **4900** |
| HNO3 | HNO3 | Nitric acid | 63 |  | 1 x 1014 |  |
| HNO4 | HNO4 | Pernitric acid | 79 |  | **39** | **8400** |
| HO2 | HO2 | Hydroperoxyl radical | 33 |  |  |  |
| IAP | HOCH2C(CH3)(OOH)CH(OH)CHO | Peroxide from HC5OO | 150 | 5 | **2.94 x102** | **5200** |
| IEPOX | C5H10O3 | Isoprene dihydroxyepoxide epoxide | 118 | 5 | 1.30 x 108 | 0 |
| IEPOXOO | C5H9O5 | RO2 from IEPOX | 149 | 5 |  |  |
| INO2 | O2NOCH2C(OO)(CH3)CH=CH2 or O2NOCH2C(CH3)=CHCH2OO | RO2 from ISOP+NO3 | 162 | 5 |  |  |
| INPN | O2NOCH2C(OOH)(CH3)CH=CH2 | Peroxide from INO2 | 163 | 5 | **2.94 x102** | **5200** |
| ISN1 | C5H7NO4 or C5H9NO4 | C5-nitrooxycarbonyl | 145/147 | 5 | 1.70 x 104 | 9200 |
| ISNOHOO | C5H8NO7 or C5H10NO7 | peroxy radical from ISN1+OH | 194/196 | 5 |  |  |
| ISNOOA | C5H6NO6 or C5H8NO6 | acyl peroxy radical from ISN1 | 176/178 | 5 |  |  |
| ISNOOB | C5H7N2O9 or C5H9N2O9 | peroxy radical from ISN1+NO3 | 239/241 | 5 |  |  |
| ISNP | HOCH2C(OOH)(CH3)CH(ONO2)CH2OH | Peroxide from ISOPNBO2 and ISOPNDO2 | 197 | 5 | **2.94 x102** | **5200** |
| ISOA11 |  | Lumped semivolatile aerosol products of isoprene oxidation | 150 | 9 | As aerosol |  |
| ISOA2 |  | Lumped semivolatile aerosol products of isoprene oxidation | 150 | 9 | As aerosol |  |
| ISOA3 |  | Lumped semivolatile aerosol products of isoprene oxidation | 150 | 9 | As aerosol |  |
| ISOG12 |  | Lumped semivolatile gas products of isoprene oxidation | 150 | 9 | 1.0 x 105 | 6039 |
| ISOG2 |  | Lumped semivolatile gas products of isoprene oxidation | 150 | 9 | 1.0 x 105 | 6039 |
| ISOG3 |  | Lumped semivolatile gas products of isoprene oxidation | 150 | 9 | 1.0 x 105 | 6039 |
| ISOP | CH2=C(CH3)CH=CH2 | Isoprene | 68 | 5 | **3.45 x10-2** | **4400** |
| ISOPND | C5H9NO4 | Delta hydroxy isoprene nitrate | 147 | 5 | 1.70 x 104 | 9200 |
| ISOPNB | C5H9NO4 | Beta hydroxy isoprene nitrate | 147 | 5 | 1.70 x 104 | 9200 |
| ISOPNBO2 | C5H10O7 | Peroxy radical from ISOPNB | 182 | 5 |  |  |
| ISOPNDO2 | C5H10O7 | Peroxy radical from ISOPND | 182 | 5 |  |  |
| KO2 | C4H7O3 | RO2 from >3 ketones | 103 | 4 |  |  |
| MACR | CH2=C(CH3)CHO | Methacrolein | 70 | 4 | **4.86** | **4300** |
| MACRN | HOCH2C(ONO2)(CH3)CHO | Nitrate from MACR | 149 | 4 | **1.70 x 104** | **9200** |
| MACRNO2 | C4H5NO5 or C4H6NO7 | Peroxy radical from MACRN+OH | 147/180 | 4 |  |  |
| MAN2 | HOCH2C(ONO2)(CH3)CHO | RO2 from MACR+NO3 | 149 | 4 |  |  |
| MAO3 | CH2=C(CH3)C(O)OO | Peroxyacyl from MVK and MACR | 101 | 4 |  |  |
| MAOP | CH2=C(CH3)C(O)OOH | Peroxide from MAO3 | 102 | 4 | **2.94 x102** | **5200** |
| MAOPO2 | CH2OH-CHOO\*CH3C(O)OOH | Peroxy radical from MAOP (addition on the double bond) | 152 | 4 |  |  |
| MAP | CH3C(O)OOH | Peroxyacetic acid | 76 | 2 | 8.4x102 | 5300 |
| MCO3 | CH3C(O)OO | Peroxyacetyl radical | 75 | 2 | **0.1** | **0** |
| MEK | C4H8O | >C3 ketones (methyl ethyl ketone) | 72 | 4 | **18.2** | **5700** |
| MGLY | CH3COCHO | Methylglyoxal | 72 | 3 | *3.24**x104* | *6200* |
| MVKN | HOCH2CH(ONO2)C(=O)CH3 | Methylvinylketone nitrate | 149 | 4 | 1.70 x104 | 9200 |
| MACRN | HOCH2C(ONO2)(CH3)CHO | Methacrolein nitrate | 149 | 4 | 1.70 x104 | 9200 |
| MO2 | CH3OO | Methylperoxy radical | 47 | 1 | **15.2** | **3700** |
| MOBA | HOC(=O)C(CH3)=CHCHO | 5C acid from isoprene | 114 | 5 | 2.60 x104 | 6300 |
| MOBAOO | C5HxOx | RO2 from MOBA |  | 5 |  |  |
| MOH | CH3OH | Methanol | 32 | 1 | **2.03** **x102** | **5600** |
| MP | CH3OOH | Methylhydroperoxide | 48 | 1 | *2.94* *x102* | *5200* |
| MPN | CH3O2NO2 | Methyl peroxide nitrate | 93 | 1 | **2.94 x102** | **5200** |
| MRO2 | HOCH2C(OO)(CH3)CHO | RO2 from MACR+OH | 119 | 4 |  |  |
| MRP | HOCH2C(OOH)(CH3)CHO | Peroxide from MRO2 | 120 | 4 |  |  |
| MSA | CH4SO3 | Methylsulfonic acid | 96 | 1 | As aerosol |  |
| MVK | CH2=CHC(O)CH3 | Methylvinylketone | 70 | 4 | 26.3 | 4800 |
| MVKN | HOCH2CH(ONO2)C(=O)CH3 | Nitrate from MVK | 149 | 4 |  |  |
| N2 | N2 | Nitrogen molecule | 28 |  |  |  |
| N2O | N2O | Nitrous acid | 44 |  |  |  |
| N2O5 | N2O5 | Dinitrogen pentoxide | 108 |  |  |  |
| NH2 | NH2 | Ammonia radical | 16 |  |  |  |
| NH3 | NH3 | Ammonia | 17 |  | 3.3 x106 | 4100 |
| NO | NO | Nitric oxide | 30 |  |  |  |
| NO2 | NO2 | Nitrogen dioxide | 46 |  |  |  |
| NO3 | NO3 | Nitrate radical | 62 |  |  |  |
| O | O | Oxygen atom (3P) | 16 |  |  |  |
| O2 | O2 | Oxygen molecule | 32 |  |  |  |
| O3 | O3 | Ozone | 48 |  | 0.01  (dry dep) |  |
| OH | OH | Hydroxyl radical | 17 |  |  |  |
| PAN | CH3C(O)OONO2 | Peroxyacetylnitrate | 121 | 2 | **2.94** | **5700** |
| PMN | CH2=C(CH3)C(O)OONO2 | Peroxymethacryloyl nitrate (MPAN) | 147 | 4 | **1.72** | **0** |
| PMNN | C4H6N2O9 | Product of MACRNO2+NO2 | 226 | 4 |  |  |
| PO2 | HOCH2CH(OO)CH3 | RO2 from propene | 91 | 3 |  |  |
| PP | HOCH2CH(OOH)CH3 | Peroxide from PO2 | 92 | 3 | **2.94 x102** | **5200** |
| PPN | CH3CH2C(O)OONO2 | peroxypropionylnitrate | 135 | 3 | **2.94** | **0** |
| PRN1 | O2NOCH2CH(OO)CH3 | RO2 from propene + NO3 | 136 | 3 |  |  |
| PROPNN | CH3C(O)CH2ONO2 | propanone nitrate | 119 | 3 | 1.00 x103 | 0 |
| PRPE | C3H6 | >=C3 alkenes | 42 | 3 | **7.40 x10-3** | **3400** |
| PRPN | O2NOCH2CH(OOH)CH3 | Peroxide from PRN1 | 137 | 3 | **2.94 x102** | **5200** |
| PYAC | CH3COCOOH | Pyruvic acid | 88 | 5 | **3.14** **x105** | **5100** |
| R4N1 | C4H8NO5 | RO2 from R4N2 | 150 | 4 |  |  |
| R4N2 | C4H9NO3 | >=C4 alkylnitrates | 119 | 4 | **1.0** | **5800** |
| R4O2 | C4H9O2 | RO2 from ALK4 | 89 | 4 |  |  |
| R4P | CH3CH2CH2CH2OOH | Peroxide from R4O2 | 90 | 4 | **2.94 x102** | **5200** |
| RA3P | CH3CH2CH2OOH | Peroxide from A3O2 | 76 | 3 | **2.94 x102** | **5200** |
| RB3P | CH3CH(OOH)CH3 | Peroxide from B3O2 | 76 | 3 | **2.94 x102** | **5200** |
| RCHO | CH3CH2CHO | >C2 aldehydes | 58 | 3 | **10.0** | **0** |
| RCO3 | CH3CH2C(O)OO | Peroxypropionyl radical | 89 | 3 |  |  |
| RCOOH | C2H5C(O)OH | >C2 organic acids | 74 | 3 | **15.2** | **6800** |
| RIO2 | HOCH2C(OO)(CH3)CH=CH2 | RO2 from isoprene (named as ISOPO2 in the literature) | 117 | 5 |  |  |
| RIP | HOCH2C(OOH)(CH3)CH=CH2 | Peroxide from RIO2 (named as ISOPOOH in the literature) | 118 | 5 | 1.70 x106 | 0 |
| ROH | C3H7OH | >C2 alcohols | 60 | 3 | **1.42** **x102** | **6900** |
| RP | CH3CH2C(O)OOH | Peroxide from RCO3 | 90 | 3 | **2.94 x102** | **5200** |
| SO2 | SO2 | Sulfur Dioxide | 64 |  | 1.0 x105 |  |
| SO4 | SO4 | Sulfate | 96 |  | As aerosol |  |
| TSOA01 |  | Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation | 150 | 11 | As aerosol |  |
| TSOA1 |  | Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation | 150 | 11 | As aerosol |  |
| TSOA2 |  | Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation | 150 | 11 | As aerosol |  |
| TSOA3 |  | Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation | 150 | 11 | As aerosol |  |
| TSOG02 |  | Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation | 150 | 11 | 1.0 x105 | 6039 |
| TSOG1 |  | Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation | 150 | 11 | 1.0 x105 | 6039 |
| TSOG2 |  | Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation | 150 | 11 | 1.0 x105 | 6039 |
| TSOG3 |  | Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation | 150 | 11 | 1.0 x105 | 6039 |
| VRO2 | HOCH2CH(OO)C(O)CH3 | RO2 from MVK+OH | 119 | 4 |  |  |
| VRP | HOCH2CH(OOH)C(O)CH3 | Peroxide from VRO2 | 120 | 4 | **2.94 x102** | **5200** |

1SOA in the main text is the sum of ASOA1-3, ISOA1-3 and TSOA0-3

2 SOG in the main text is the sum of ASOG1-3, ISOG1-3 and TSOG0-3

**Table 2.** List of reactions included in the GEOS-Chem standard chemical mechanism. Added chemistry to the standard mechanism is not listed here but can be found in *Fisher et al.,* [2016] for monoterpene chemistry, *Knote et al.,* [2014] for aromatics and MBO chemistry, C2H2 and C2H4 from *Lamarque et al.,* [2012]. *Troe* refers to pressure dependent reactions that follows the Troe parameterization

|  |  |
| --- | --- |
| **Reaction** | **K=Aexp(B/T) [cm3 molec−1 s−1]** |
| O3 +NO→NO2 +O2 | 3E-12 exp(-1500/T) |
| O3 +OH→HO2 +O2 | 1.7E-12 exp(-940/T) |
| O3 +HO2→OH +O2 +O2 | 1E-14 exp(-490/T) |
| O3 +NO2→O2 +NO3 | 1.2E-13 exp(-2450/T) |
| O3 +MO2→CH2O +HO2 +O2 | 2.9E-16 exp(-1000/T) |
| OH +OH→H2O +O3 | 1.8E-12 |
| OH +OH +M→H2O2 | Troe: ko=6.9E-31(300/T); ki=2.6E-11; f=0.6 |
| OH +HO2→H2O +O2 | 4.8E-11 exp(250/T) |
| OH +H2O2→H2O +HO2 | 1.8E-12 |
| HO2 +NO→OH +NO2 | 3.3E-12 exp(270/T) |
| HO2 +HO2→H2O2  HO2+HO2+M→H2O2 | k1=3E‐13 exp(460/T); k2=2.10E‐33 [M]exp(920/T)  k→ (k1 + k2)\*(1+1.4E‐ 21\*[H2O])\*exp(2200/T) |
| OH +H2→H2O +HO2 | 2.8E-12 exp(-1800/T) |
| CO +OH→HO2 +CO2 | 1.5E-13 |
| OH +CH4→MO2 +H2O | 2.45E-12 exp(-1775/T) |
| MO2 +NO→CH2O +HO2 +NO2 | 2.8E-12 exp(300/T) |
| MO2 +HO2→MP +O2 | 4.1E-13 exp(750/T) |
| MO2 +MO2→MOH +CH2O +O2 | k1=9.5E-14 exp(390/T); k2=2.62E+1 exp(-1130/T); k=k1 / (1+k2) |
| MO2 +MO2→2CH2O +2HO2 | k1=9.5E-14 exp(390/T); k2=4E-02 exp(1130/T); K=k1 / (1+k2) |
| MP +OH→MO2 +H2O | 2.66E-12 exp(200/T) |
| MP +OH→CH2O +OH +H2O | 1.14E-12 exp(200/T) |
| ATOOH +OH→ATO2 +H2O | 2.66E-12 exp(200/T) |
| ATOOH +OH→MGLY +OH +H2O | 1.14E-12 exp(200/T) |
| CH2O +OH→CO +HO2 +H2O | 5.5E-12 exp(125/T) |
| NO2 +OH +M→HNO3 +M | Troe: ko=1.80E-30(300/T)3; ki=2.80E‐11(300/T); fc=0.6 |
| HNO3 +OH→H2O +NO3 | k0=2.41E-14 exp(460/T); k2=2.69E-17exp(2199/T);  k3=6.51E-34exp(1335/T); k=k0 + k3[M] / (1 + k3[M]/k2) |
| NO +OH +M→HNO2 +M | Troe: ko: 7.00E-31(300/T)2.6; ki: 3.60E-11(300/T)0.1; fc= 0.6 |
| HNO2 +OH→H2O +NO2 | 1.8E-11 exp(-390/T) |
| HO2 +NO2 +M→HNO4 +M | Troe: ko= 2E‐31(300/T)3.4; ki=2.9E‐12(300/T)1.1; fc= 0.6 |
| HNO4 +M→HO2 +NO2 | Troe: ko= 9.52E‐5(300/T)3.4 exp(‐ 10900/T); ki=1.38E+15\*(300/T)1.1exp(‐ 10900/T); fc= 0.6 |
| HNO4 +OH→H2O +NO2 +O2 | 1.3E-12 exp(380/T) |
| HO2 +NO3→OH +NO2 +O2 | 3.5E-12 |
| NO +NO3→2NO2 | 1.5E-11 exp(170/T) |
| OH +NO3→HO2 +NO2 | 2.2E-11 |
| NO2 +NO3 +M→N2O5 +M | Troe: ko= 2E-30(300/T)4.4; ki=1.4E-12(300/T)0.7; fc= 0.6 |
| N2O5 +M→NO2 +NO3 | Troe: k0= 7.4E-04(300/T)4.4 exp(-11000/T);  ki=5.18E+14(300/T)0.7 exp(-11000/T); fc= 0.6 |
| HCOOH +OH→H2O +CO2 +HO2 | 4E-13 |
| MOH +OH→HO2 +CH2O | 2.9E-12 exp(-345/T) |
| NO2 +NO3→NO +NO2 +O2 | 4.5E-14 exp(-1260/T) |
| NO3 +CH2O→HNO3 +HO2 +CO | 5.8E-16 |
| ALD2 +OH→0.95MCO3 +0.05CH2O +0.05CO+0.05HO2 | 4.63E-12 exp(350/T) |
| ALD2 +NO3→HNO3 +MCO3 | 1.4E-12 exp(-1900/T) |
| MCO3 +NO2 +M→PAN | Troe: ko= 9.7E-29(300/T)5.6; ki=9.3E-12(300/T)1.5; fc= 0.6 |
| PAN →MCO3 +NO2 | 9.3E-29 exp(14000/T) |
| MCO3 +NO→MO2 +NO2 +CO2 | 8.1E-12 exp(270/T) |
| C2H6 +OH→ETO2 +H2O | 7.66E-12 exp(-1020/T) |
| ETO2 +NO→ALD2 +NO2 +HO2 | 2.6E-12 exp(365/T) |
| C3H8 +OH→B3O2 | k1=7.6E-12 exp(-585/T); k2=5.87\*(300/T)0.64 exp(‐ 816/T);  K=k1 / (1+k2) |
| C3H8 +OH→A3O2 | k1=7.60E‐12 exp(‐585/T); k2= 0.17\*(300/T)‐0.64 exp(816/T)  K=k1 / (1+k2) |
| A3O2 +NO→NO2 +HO2 +RCHO | 2.9E-12 exp(350/T) |
| PO2 +NO→NO2 +HO2 +CH2O +ALD2 | 2.7E-12 exp(350/T) |
| ALK4 +OH→R4O2 | 9.1E-12 exp(-405/T) |
| R4O2 +NO→NO2 +0.32ACET +0.19MEK +0.18MO2 +  0.27HO2 +0.32ALD2 +0.13RCHO+0.05A3O2 +0.093B3O2 +0.32ETO2 | 2.7E-12 exp(350/T) |
| R4O2 +NO→R4N2 | 2.7E-12 exp(350/T) |
| R4N1 +NO→2NO2 +0.570RCHO +0.86 ALD2+0.57CH2O | 2.7E-12 exp(350/T) |
| ATO2 +NO→NO2 +CH2O +MCO3 | 2.8E-12 exp(300/T) |
| KO2 +NO→0.93NO2 +0.93ALD2 +0.93MCO3 +0.07R4N2 | 2.7E-12 exp(350/T) |
| RIO2 +NO→0.883NO2 +0.783HO2 +0.66CH2O +0.4MVK+0.26MACR+0.07ISOPND+0.047ISOPNB+0.123HC5 +0.1DIBOO | 2.7E-12 exp(350/T) |
| RIO2 →2HO2+0.5MGLY +0.5GLYC+0.5GLYX +0.5HAC+OH | 4.07E+08 exp(-7694/T) |
| VRO2 +NO→0.88NO2 +0.35HO2 +0.35CH2O+0.53MCO3 +0.53GLYC +0.35MGLY +0.12MVKN | 2.7E-12 exp(350/T) |
| MRO2 +NO→0.8NO2 +0.8HO2 +0.1MGLY +0.7HAC  +0.7CO +0.1CH2O +0.1MACRN | 2.7E-12 exp(350/T) |
| MRO2 →CO +HAC +OH | 2.9E+07 exp(-5297/T) |
| MAN2 +NO→1.5NO2 +0.5CH2O +0.5MGLY  +0.5PROPNN+0.5CO +0.5OH | 2.7E-12 exp(350/T) |
| B3O2 +NO→NO2 +HO2 +ACET | 2.7E-12 exp(350/T) |
| INO2 +NO→1.3NO2 +0.8HO2 +0.7ISN1 +0.23HC5  +0.035MACR +0.07CH2O +0.035MVK | 2.7E-12 exp(350/T) |
| INO2 +NO3→1.3NO2 +0.8HO2 +0.7ISN1 +0.23HC5  +0.035MACR +0.07CH2O +0.035MVK | 2.3E-12 |
| ISN1 +NO3→0.6ISNOOA+0.4ISNOOB+0.6HNO3 | 3.15E-13 exp(-448/T) |
| ISNOOA+NO3→NO2 +R4N2 +CO +HO2 | 4E-12 |
| ISNOOA+NO→NO2 +R4N2 +CO +HO2 | 6.7E-12 exp(340/T) |
| ISNOOA+NO2→PMN +{CO2}1 | Troe: ko= 9.0E-28(300/T)8.9; ki=7.7E-12(300/T)0.2; fc=0.6 |
| ISNOOA+HO2→0.75RP +0.25RCOOH +0.25O3 +2{CO2} | 5.2E-13 exp(980/T) |
| ISNOOB+NO3→PROPNN +GLYX +2NO2 | 2.3E-12 |
| ISNOOB+NO→0.06R4N2 + 0.94PROPNN +0.94GLYX +1.88NO2 | 2.6E-12 exp(380/T) |
| ISNOOB+HO2→INPN | 2.06E-13 exp(1300/T) |
| ISNOOB+MO2→0.7R4N2 +0.7GLYX +0.7NO2 +0.25CH2O +0.25MOH +0.5HO2 +0.5CH2O +0.8{CO2} | 2E-13 |
| ISN1 +O3→0.3R4N2 +0.7GLYX +0.7NO2 +0.25CH2O  +0.25MOH +0.5HO2 +0.5CH2O +1.4{CO2} | 4.15E-15 exp(-1520/T) |
| ISN1 +OH→0.345ISNOOA+0.655ISNOHOO | 7.48E-12 exp(410/T) |
| ISNOHOO+NO→0.081R4N2 + 0.919PROPNN +0.934HO2 +0.919GLYX | 2.6E-12 exp(380/T) |
| ISNOHOO+HO2→INPN | 2.06E-13 exp(1300/T) |
| ISNOHOO+MO2→0.7R4N2 +0.7GLYX +0.7HO2  +0.25CH2O +0.25MOH +0.5CH2O +0.5HO2 +0.8{CO2} | 2.06E-13 |
| INO2 +INO2→0.3NO2 +0.8HO2 +0.7ISN1 +0.23HC5  +0.035MACR +0.07CH2O +0.035MVK +0.5ISN1+0.5ISOPND | 1.2E-12 |
| PRN1 +NO→2NO2 +CH2O +ALD2 | 2.7E-12 exp(350/T) |
| ALK4 +NO3→HNO3 +R4O2 | 2.8E-12 exp(-3280/T) |
| R4N2 +OH→R4N1 +H2O | 1.6E-12 |
| ACTA +OH→MO2 +CO2 +H2O | 3.15E-14 exp(920/T) |
| OH +RCHO→RCO3 +H2O | 6.0E-12 exp(410/T) |
| RCO3 +NO2 +M→PPN | Troe: ko=9E-28(300/T)8.9; ki=7.7E-12(300/T)0.2; fc=0.6 |
| PPN→RCO3 +NO2 | 9.0E-29 exp(14000/T) |
| MAO3 +NO2 +M→PMN | Troe: ko=9E-28(300/T)8.9; ki=7.7E-12(300/T)0.2; fc=0.6 |
| PMN →MAO3 +NO2 | 9.0E-29 exp(14000/T) |
| RCO3 +NO→NO2 +ETO2 +{CO2} | 6.7E-12 exp(340/T) |
| MAO3 +NO→1NO2 +0.5CH2O +0.5CO +CO2  +0.5MO2 +0.5MCO3 +0.5{CO2} | 6.7E-12 exp(340/T) |
| RCHO +NO3→HNO3 +RCO3 | 6.5E-15 |
| ACET +OH→ATO2 +H2O | 1.33E-13 |
| ACET +OH→ATO2 +H2O | 3.82E-11 exp(-2000/T) |
| A3O2 +MO2→HO2 +0.75CH2O +0.75RCHO  +0.25MOH +0.25ROH | 5.92E-13 |
| PO2 +MO2→HO2 +0.5ALD2 +1.25CH2O +0.16HAC  +0.09RCHO +0.25MOH +0.25ROH | 5.92E-13 |
| R4O2 +HO2→R4P | 7.4E-13 exp(700/T) |
| R4N1 +HO2→R4N2 | 7.4E-13 exp(700/T) |
| ATO2 +HO2→0.15MCO3 +0.15OH +0.15CH2O +0.85ATOOH | 8.6E-13 exp(700/T) |
| KO2 +HO2→0.15OH +0.15ALD2 +0.15MCO3 +0.85ATOOH +0.85{CO2} | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| RIO2 +HO2→0.88RIP +0.12OH +0.047MACR +0.073MVK +0.12HO2+0.12CH2O | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=5 |
| VRO2 +HO2→0.1VRP +0.68OH +0.578GLYC +0.578MCO3+0.187MEK +0.102HO2 +0.102CH2O +0.102MGLY +0.033RCHO +0.033{CO2} | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| MRO2 +HO2→MRP | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| MAN2 +HO2→0.075PROPNN+0.075CO +0.075HO2 +0.075MGLY+0.075CH2O +0.075NO2 +0.15OH +0.85MAOP + 0.85NO2 | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)],n=4 |
| B3O2 +HO2→RB3P | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)],n=3 |
| INO2 +HO2→INPN | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)],n=5 |
| PRN1 +HO2→PRPN | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)],n=3 |
| MEK +OH→KO2 +H2O | 1.3 E‐12exp(‐25/T) |
| MO2 +ETO2→0.75CH2O +0.75ALD2 +HO2 +0.25MOH +0.25EOH | 3E-13 |
| MEK +NO3→HNO3 +KO2 | 8.0E-16 |
| R4O2 +MO2→0.16ACET +0.1MEK +0.09MO2 +0.14HO2+0.16ALD2 +0.07RCHO +0.03A3O2 +0.09B3O2 +0.16ETO2+0.25MEK +0.75CH2O +0.25MOH +0.25ROH +0.5HO2 +0.07{CO2} | 8.37E-14 |
| R4N1 +MO2→NO2 +0.2CH2O +0.38ALD2  +0.29RCHO +0.15R4O2 +0.25RCHO +0.75CH2O  +0.25MOH +0.25ROH +0.5HO2 +0.07{CO2} | 8.37E-14 |
| ATO2 +MO2→0.3HO2 +0.3CH2O +0.3MCO3  +0.2HAC +0.2CH2O +0.5MGLY +0.5MOH +0.3{CO2} | 7.5E-13 exp(500/T) |
| KO2 +MO2→0.5ALD2 +0.5MCO3 +0.25MEK  +0.75CH2O +0.25MOH +0.25ROH +0.5HO2 +0.25{CO2} | 8.37E-14 |
| RIO2 +MO2→1.1HO2 +1.22CH2O +0.28MVK  +0.18MACR +0.3HC5 +0.24MOH +0.24ROH +0.48{CO2} | 8.37E-14 |
| RIO2 +RIO2→1.28HO2 +0.92CH2O +0.56MVK  +0.36MACR +0.48ROH +0.5HC5 +1.46{CO2} | 1.54E-13 |
| HC5OO +MO2→0.5HO2 +0.33CO +0.09H2  +0.18HAC +0.13GLYC +0.29MGLY +0.25MEK +0.95CH2O+0.25MOH +0.25ROH +0.5HO2 +1.05{CO2} | 8.37E-14 |
| VRO2 +MO2→0.14HO2 +0.14CH2O +0.36MCO3  +0.36GLYC +0.14MGLY +0.25MEK +0.75CH2O +0.25MOH+0.25ROH +0.5HO2 +0.25{CO2} | 8.37E-14 |
| MRO2 +MO2→0.595HAC +0.255MGLY +0.595CO +1.255CH2O+1.7HO2 +0.15ROH +0.15{CO2} | 8.37E-14 |
| MAN2 +MO2→0.375PROPNN+0.375CO +0.375HO2 +0.375MGLY+0.375CH2O +0.375NO2 +0.25CH2O +0.25R4N2 +0.75{CO2} | 8.37E-14 |
| B3O2 +MO2→0.5HO2 +0.5ACET +0.25ACET +0.75CH2O+0.25MOH +0.25ROH +0.5HO2 +0.021{CO2} | 8.37E-14 |
| INO2 +MO2→0.15NO2 +0.4HO2 +0.35ISN1 +0.035CH2O+0.018MACR +0.018MVK +0.115HC5 +0.25ISN1 +0.25ISOPND+0.5CH2O +0.5HO2 +0.25CH2O +0.25MOH | 1.3E-12 |
| PRN1 +MO2→NO2 +0.5CH2O +0.5ALD2 +0.25RCHO +0.75CH2O +0.25MOH +0.25ROH +0.5HO2 | 8.37E-14 |
| EOH +OH→HO2 +ALD2 | 3.35E-12 |
| ROH +OH→HO2 +RCHO | 4.6E-12 exp(70/T) |
| ETO2 +ETO2→2ALD2 +2HO2 | 4.1E-14 |
| ETO2 +ETO2→EOH +ALD2 | 2.7E-14 |
| HO2 +ETO2→ETP | 7.4E-13 exp(700/T) |
| A3O2 +HO2→RA3P | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=3 |
| PO2 +HO2→PP | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)]; n=3 |
| HO2 +MCO3→0.41MAP +0.15ACTA +0.15O3 +0.44OH+0.44MO2 +0.44{CO2} | 5.2E-13 exp(980/T) |
| RCO3 +HO2→0.41RP +0.15RCOOH +0.15O3 +0.44OH +0.44ETO2 +0.44{CO2} | 4.3E-13 exp(1040/T) |
| MAO3 +HO2→0.44OH +0.15O3 +0.59CH2O +0.39MO2 +0.41MAOP +0.39CO +0.99{CO2} | 4.3E-13exp(1040/T) |
| PRPE +OH +M→PO2 | Troe: ko=8.0E-27(300/T)3.5; ki=3E-11(300/T); fc=0.6 |
| PRPE +O3→0.4ALD2 +0.244OH +0.244HO2 +0.42CO +0.58CH2O +0.148HCOOH +0.096ACTA +0.036MOH +0.824{CO2} | 5.5E-15 exp(-1880/T) |
| PMN +OH→HAC +CO +NO2 | 2.9E-11 |
| PMN +O3→NO2 +0.6CH2O +HO2 +3.4{CO2} | 8.2E-18 |
| GLYC +OH→0.732CH2O +0.361CO2 +0.505CO +0.227OH+0.773HO2 +0.134GLYX +0.134HCOOH | 8.0E-12 |
| GLYC +OH→HCOOH +OH +CO | 8.0E-12 |
| PRPE +NO3→PRN1 | 4.59E-13 exp(-1156/T) |
| GLYX +OH→HO2 +2CO | 3.1E-12 exp(340/T) |
| MGLY +OH→MCO3 +CO | 1.5E-11 |
| GLYX +NO3→HNO3 +HO2 +2CO | 1.4E-12 exp(-1860/T) |
| MGLY +NO3→HNO3 +CO +MCO3 | 3.36E-12 exp(-1860/T) |
| ISOP +OH→RIO2 | 3.1E-11 exp(350/T) |
| MVK +OH→VRO2 | 2.6E-12 exp(610/T) |
| MACR +OH→0.53MAO3 +0.47MRO2 | 8.0E-12 exp(380/T) |
| HAC +OH→MGLY +HO2 | 2.15E-12 exp(305/T) |
| HAC +OH→0.5HCOOH +OH +0.5ACTA +0.5CO2 +0.5CO +0.5MO2 | 2.15E-12 exp(305/T) |
| MCO3 +A3O2→MO2 +RCHO +HO2 +{CO2} | 1.68E-12 exp(500/T) |
| MCO3 +PO2→MO2 +ALD2 +CH2O +HO2+{CO2} | 1.68E-12 exp(500/T) |
| MCO3 +A3O2→ACTA +RCHO | 1.87E-13 exp(500/T) |
| MCO3 +PO2→1ACTA +0.35RCHO +0.65HAC | 1.87E-13 exp(500/T) |
| ISOP +O3→0.244MVK +0.325MACR +0.845CH2O +0.11H2O2 +0.522CO +0.204HCOOH +0.199MCO3 +0.026HO2+0.27OH +0.128PRPE +0.051MO2 +0.32{CO2} | 1E-14 exp(-1970/T) |
| MVK +O3→0.202OH +0.202HO2 +0.352HCOOH +0.535CO+0.05ALD2 +0.95MGLY +0.05CH2O +0.113{CO2} | 8.5E-16 exp(-1520/T) |
| MACR +O3→0.3OH +0.2HO2 +0.3HCOOH +0.6CO  +0.9MGLY +0.1CH2O +0.3CO2 | 1.4E-15 exp(-2100/T) |
| ISOP +NO3→INO2 | 3.3E-12 exp(-450/T) |
| MACR +NO3→MAN2 | 2.3E-15 |
| MACR +NO3→MAO3 +HNO3 | 1.1E-15 |
| RCO3 +MO2→CH2O +HO2 +ETO2 | 1.68E-12 exp(500/T) |
| MAO3 +MO2→CH2O +HO2 +CH2O +MCO3 +{CO2} | 1.68E-12 exp(500/T) |
| RCO3 +MO2→RCOOH +CH2O | 1.87E-13 exp(500/T) |
| MAO3 +MO2→RCOOH +CH2O +{CO2} | 1.87E-13 exp(500/T) |
| INPN +OH→OH +NO2 +MEK +{CO2} | 1.9E-11 exp(390/T) |
| INPN +OH→0.36INO2 +0.64R4N2 +0.64OH +0.64{CO2} | 5.18E-12 exp(200/T) |
| PRPN +OH→0.209PRN1 +0.791OH +0.791PROPNN | 8.78E-12 exp(200/T) |
| ETP +OH→0.64OH +0.36ETO2 +0.64ALD2 | 5.18E-12 exp(200/T) |
| RA3P +OH→0.64OH +0.36A3O2 +0.64RCHO | 5.18E-12 exp(200/T) |
| RB3P +OH→0.791OH +0.209B3O2 +0.791ACET | 8.78E-12 exp(200/T) |
| R4P +OH→0.791OH +0.209R4O2 +0.791RCHO +0.791{CO2} | 8.78E-12 exp(200/T) |
| RP +OH→RCO3 | 6.13E-13 exp(200/T) |
| PP +OH→0.791OH +0.209PO2 +0.791HAC | 8.78E-12 exp(200/T) |
| RIP +OH→0.387RIO2 +0.613OH +0.613HC5 | 4.75E-12 exp(200/T) |
| RIP +OH→OH +IEPOX | 1.9E-11 exp(390/T) |
| IEPOX +OH→IEPOXOO | 5.78E-11 exp(-400/T) |
| EPOXOO + HO2 = 0.725HAC + 0.275GLYC + 0.275GLYX + 0.275MGLY + 1.125OH + 0.825HO2 + 0.200CO2 + 0.375CH2O + 0.074HCOOH + 0.251CO | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=5 |
| IEPOXOO + NO → 0.725HAC+0.275GLYC+ 0.275GLYX +0.275MGLY +0.125OH +0.825HO2+0.200CO2+0.375CH2O +0.074HCOOH +0.251CO +NO2 | 2.7E-12 exp(350/T) |
| IAP +OH→0.654OH +0.654DHMOB +0.346HC5OO | 5.31E-12 exp(200/T) |
| VRP +OH→0.791OH +0.791MEK+0.209VRO2 | 8.78E-12 exp(200/T) |
| MRP +OH→MRO2 | 1.84E-12 exp(200/T) |
| MRP +OH→CO2 +HAC +OH | 4.4E-12 exp(380/T) |
| MAOP +OH→MAO3 | 6.13E-13 exp(200/T) |
| MAOP +OH→MAOPO2 | 3.6E-12 exp(380/T) |
| MCO3 +MAOPO2+→HAC +2CO2 +OH+MO2 | 1.68E-12 exp(500/T) |
| MCO3 +MAOPO2+→ACTA +MEK | 1.87E-13 exp(500/T) |
| MAOPO2+MO2 +→0.7HAC +0.7CO2 +0.7OH +CH2O+0.7HO2 +0.3ROH+0.3{CO2} | 8.37E-14 |
| MAOPO2+MAOPO2+→2HAC +2CO2 +2OH | 8.37E-14 |
| MAOPO2+HO2→HAC +CO2 +2OH | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| MAOPO2+NO→HAC +CO2 +OH +NO2 | 2.7E-12 exp(350/T) |
| MAOPO2+NO→HNO3 +4{CO2} | 2.7E-12 exp(350/T) |
| OH +MAP→MCO3 | 6.13E-13 exp(200/T) |
| C2H6 +NO3→ETO2 +HNO3 | 1.4E-18 |
| HC5 +O3→0.6MGLY +0.1OH +0.12CH2O +0.28GLYC +0.3O3 +0.4CO +0.2H2 +0.2HAC +0.2HCOOH +1.32{CO2} | 6.16E-15 exp(-1814/T) |
| MCO3 +MCO3→2MO2 +2{CO2} | 2.5E-12 exp(500/T) |
| MCO3 +MO2→CH2O +MO2 +1HO2 +1CO2 | 1.8E-12 exp(500/T) |
| MCO3 +MO2→ACTA +CH2O | 2E-13 exp(500/T) |
| R4O2 +MCO3→MO2 +0.32ACET +0.19MEK  +0.27HO2 +0.32ALD2 +0.13RCHO +0.05A3O2 +0.18B3O2+0.32ETO2 +0.92{CO2} | 1.68E-12 exp(500/T) |
| ATO2 +MCO3→MO2 +MCO3 +CH2O +{CO2} | 1.68E-12 exp(500/T) |
| KO2 +MCO3→MO2 +ALD2 +MCO3 +{CO2} | 1.68E-12 exp(500/T) |
| RIO2 +MCO3→0.887HO2 +0.747CH2O +0.453MVK +0.294MACR+0.14HC5 +0.113DIBOO +CO2 +MO2 +0.18{CO2} | 1.68E-12 exp(500/T) |
| HC5OO +MCO3→0.216GLYX +0.234MGLY +0.234GLYC+0.216HAC +0.29DHMOB +0.17MOBA +0.09RCHO +HO2 +0.09CO +MO2 +1.09{CO2} | 1.68E-12 exp(500/T) |
| VRO2 +MCO3→0.4HO2 +0.4CH2O+ 0.6MCO3 +0.6GLYC +0.4MGLY +MO2 +{CO2} | 1.68E-12 exp(500/T) |
| MRO2 +MCO3→0.85HO2 +0.143MGLY +0.857HAC +0.857CO +0.143CH2O +MO2 +{CO2} | 1.68E-12 exp(500/T) |
| B3O2 +MCO3→MO2 +HO2 +ACET +{CO2} | 1.68E-12 exp(500/T) |
| R4N1 +MCO3→1MO2 +1NO2 +0.39CH2O  +0.75ALD2 +0.57RCHO +0.3R4O2 +0.2{CO2} | 1.68E-12 exp(500/T) |
| MAN2 +MCO3→0.5PROPNN+0.5CO +0.5HO2 +0.5MGLY +0.5CH2O +0.5NO2 +CO2 +MO2 | 1.68E-12 exp(500/T) |
| INO2 +MCO3→MO2 +0.7ISN1 +0.8HO2 +0.035MVK +0.035MACR +0.07CH2O +0.3NO2 +0.23HC5 +{CO2} | 1.68E-12 exp(500/T) |
| PRN1 +MCO3→MO2 +NO2 +CH2O +ALD2 +{CO2} | 1.68E-12 exp(500/T) |
| R4O2 +MCO3→MEK +ACTA | 1.87E-13 exp(500/T) |
| ATO2 +MCO3→MGLY +ACTA | 1.87E-13 exp(500/T) |
| KO2 +MCO3→MEK +ACTA | 1.87E-13 exp(500/T) |
| RIO2 +MCO3→MEK +ACTA +{CO2} | 1.87E-13 exp(500/T) |
| HC5OO +MCO3→MEK +ACTA +{CO2} | 1.87E-13 exp(500/T) |
| VRO2 +MCO3→MEK +ACTA | 1.87E-13 exp(500/T) |
| MRO2 +MCO3→MEK +ACTA | 1.87E-13 exp(500/T) |
| R4N1 +MCO3→RCHO +ACTA +NO2 +{CO2} | 1.87E-13 exp(500/T) |
| MAN2 +MCO3→RCHO +ACTA +NO2 +{CO2} | 1.87E-13 exp(500/T) |
| INO2 +MCO3→RCHO +ACTA +NO2 +2{CO2} | 1.87E-13 exp(500/T) |
| PRN1 +MCO3→RCHO +ACTA +NO2 | 1.87E-13 exp(500/T)) |
| B3O2 +MCO3→ACET +ACTA | 1.87E-13 exp(500/T) |
| MCO3 +ETO2→MO2 +ALD2 +HO2 +{CO2} | 1.68E-12 exp(500/T) |
| MCO3 +ETO2→ACTA +ALD2 | 1.87E-13 exp(500/T) |
| RCO3 +MCO3→MO2 +ETO2 +2{CO2} | 2.5E-12 exp(500/T) |
| MAO3 +MCO3→MO2 +CH2O +MCO3 +2{CO2} | 2.5E-12 exp(500/T) |
| NO3 +NO3→2NO2 +O2 | 8.5E-13 exp(-2450/T) |
| MO2 +NO2 +M→MPN +M | Troe: ko=1E-30 (300/T)4.8; ki=7.2E-12 (300/T)2.1; fc=0.6 |
| MPN +M→MO2 +NO2 | Troe: ko= 1.1E-02(300/T)4.8 exp(-11234/T)  ki=7.6E+16 (300/T)2.1 exp(-11234/T); fc= 0.6 |
| ISOPNB+O3→0.61MVKN +0.39MACRN +0.27OH +CH2O | 1.06E-16 |
| ISOPND+O3→0.5PROPNN+0.5ETHLN +0.27OH +0.5GLYC +0.5HAC | 5.3E-17 |
| HO2 🡪 | 3.3E+01; γ2 =0.20 |
| NO2→0.5HNO3 +0.5HNO2 | 4.6E+01; γ =1E-4 |
| NO3→HNO3 | 6.2E+01; γ =0.10 |
| N2O5→2HNO3 | 1.08E+02; γ =0.10 |
| DMS +OH →SO2 +MO2 +CH2O | 1.2E-11 exp(-280/T) |
| DMS +OH +O2→0.75SO2 +0.25MSA +MO2 +0.75{CO2} | k1=8.2E-39exp(5376/T); k2=1E-05exp(3644/T); k=k1\*[O2]/(1+k2\*[O2]) |
| DMS +NO3 +→SO2 +HNO3 +MO2 +CH2O | 1.9E-13exp(530/T) |
| SO2 +OH +M→SO4 +HO2 | Troe: ko= 3.3E-31(300/T)4.3; ki=1.6E-12; fc= 0.6 |
| Br +O3→BrO +O2 | 1.7E-11 exp(-800/T) |
| BrO +HO2→HOBr +O2 | 4.5E-12 exp(460/T) |
| Br +HO2→HBr +O2 | 4.8E-12 exp(-310/T) |
| HBr +OH→Br +H2O | 5.5E-12exp(200/T) |
| BrO +BrO→2Br +O2 | 2.4E-12exp(40/T) |
| BrO +BrO→Br2 +O2 | 2.8E-14 exp(860/T) |
| BrO +NO→Br +NO2 | 8.8E-12 exp(260/T) |
| Br +BrNO3→Br2 +NO3 | 4.9E-11 |
| Br2 +OH→ HOBr +Br | 2.1E-11 exp(240/T) |
| BrO +OH→Br +HO2 | 1.7E-11 exp(250/T) |
| Br +NO3→BrO +NO2 | 1.6E-11 |
| Br +CH2O→HBr +HO2 +CO | 1.7E-11 exp(-800/T) |
| Br +ALD2→HBr +MCO3 | 1.3E-11 exp(-360/T) |
| Br +ACET→HBr +ATO2 | 1.66E-10exp(-7000/T) |
| Br +C2H6→HBr +ETO2 | 2.36E-10 exp(-6411/T) |
| Br +C3H8→HBr +A3O2 | 8.77E-11 exp(-4330/T) |
| Br +NO2 +M→BrNO2 | Troe: ko= 4.2E-31(300/T)2.4; ki=2.7E-11; fc= 0.6 |
| BrO +NO2 +M→BrNO3 | Troe: ko= 5.2E-31(300/T)3.2; ki=6.9E-12(300/T)2.9; fc= 0.6 |
| CHBr3 +OH→3Br +{CO2} | 1.35E-12 exp(-600/T) |
| CH2Br2+OH→2Br +{CO2} | 2E-12 exp(-840/T) |
| CH3Br +OH→1Br +{CO2} | 2.35E-12 exp(-1300/T) |
| BrNO3→HOBr +HNO3 | 1.42E+02; γ =0.30 |
| HOBr→0.5Br2 +H2O | 9.7E+01; γ =0.20 |
| HBr→0.5Br2 | 8.1E+01; γ =0.20 |
| HOBr→0.5Br2 +H2O | 9.7E+01; γ =0.10 |
| HBr→0.5Br2 | 8.1E+01; γ =0.10 |
| HC5 +OH→HC5OO | 3.35E-11 exp(380/T) |
| HC5OO +NO→NO2 +0.216GLYX +0.234MGLY +0.234GLYC+0.216HAC +0.29DHMOB +0.17MOBA +0.09RCHO +HO2 +0.09CO +0.09{CO2} | 2.7E-12 exp(350/T) |
| HC5OO +NO→HNO3 +5{CO2} | 2.7E-12 exp(350/T) |
| HC5OO +HO2→0.1IAP +0.9OH +0.9MGLY +0.9GLYC +0.9HO2 +1.85{CO2} | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)]; n=5 |
| ISOPND+OH→ISOPNDO2 | 2.6E-11 exp(380/T) |
| ISOPNB+OH→ISOPNBO2 | 3.6E-12 exp(380/T) |
| ISOPNDO2 + NO→ 0.070MACRN + 0.310HCOOH + 0.440HAC + 0.130ETHLN + 0.650CH2O + 1.340NO2 + 0.150GLYC + 0.310NO3 + 0.150PROPNN + 0.340MEK + 0.350HO2+0.07{CO2} | 2.7E-12 exp(350/T) |
| ISOPNDO2+NO→HNO3 +5{CO2} | 2.7E-12 exp(350/T) |
| ISOPNDO2+HO2→0.035MACRN +0.155HCOOH +0.22HAC +0.065ETHLN +0.325CH2O +0.17NO2 +0.075GLYC +0.155NO3 +0.075PROPNN+0.17MEK +0.2HO2 +0.5OH +0.5ISNP +0.035{CO2} | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)], n=5 |
| ISOPNBO2 + NO→ 0.6GLYC + 0.6HAC + 0.4CH2O + 1.6NO2 + 0.26MACRN + 0.4HO2 + 0.14MVKN | 2.7E-12 exp(350/T) |
| ISOPNBO2+NO→HNO3 +5CO2 | 2.7E-12 exp(350/T) |
| ISOPNBO2+HO2→0.3GLYC +0.3HAC +0.2CH2O +0.13MACRN +0.07MVKN +0.3NO2 +0.2HO2 +0.5OH +0.5ISNP | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)], n=5 |
| ISNP + OH→0.612OH+0.612R4N1+0.193ISOPNBO2  +0.193ISOPNDO2+0.622{CO2} | 4.75E-12exp(200/T) |
| MVKN + OH→ 0.650HCOOH+ NO3+0.650MGLY+ 0.350CH2O+0.350PYAC | 1.5E-12exp(380/T) |
| MACRN +OH→MACRNO2 | 1.39E-11exp(380/T) |
| MACRNO2 + NO→ 0.08ACTA + 0.08CH2O + 0.15NO3 + 0.07HCOOH + 0.07MGLY + 0.85HAC + 0.85NO2 + 0.93CO2 + NO2 | 2.7E-12exp(350/T) |
| MACRNO2+HO2 →0.08ACTA +0.08CH2O +0.15NO3  +0.07HCOOH +0.07MGLY +0.85HAC +0.85NO2 +0.93CO2 +OH | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| MACRNO2+NO2 +M→PMNN | Troe: ko= 9.00E-28(300/T)8.9; ki=7.70E-12(300/T)0.2; fc: 0.6 |
| PMNN→MACRNO2+NO2 | 9e-29exp(14000/T) |
| DHMOB +OH→1.5CO +1HO2 +0.5HAC +0.5MEK | 2.52E-11exp(410/T) |
| DIBOO + NO→HO2+NO2+0.520GLYC +0.520MGLY +0.480HAC+0.480GLYX | 2.7E-12 exp(350/T) |
| DIBOO +NO→HNO3 +5{CO2} | 2.7E-12 exp(350/T) |
| DIBOO +HO2→0.15HO2 +0.15OH +0.078GLYC+  0.078MGLY+0.072HAC +0.072GLYX +0.85R4P +0.85{CO2} | 2.91E-13\*exp(1300/T)[1-exp(-0.245\*n)], n=5 |
| MOBA +OH→MOBAOO | 7.9E-12 exp(380/T) |
| MOBAOO+NO →RCHO +CO2 +HO2 +NO2 +{CO2} | 2.7E-12 exp(350/T) |
| MOBAOO+NO +→1HNO3 +5{CO2} | 2.7E-12 exp(350/T) |
| MOBAOO+HO2 →0.5OH +0.5HO2 +0.5RCHO +0.5CO2 +0.5R4P +{CO2} | 2.91E-13exp(1300/T)[1-exp(-0.245\*n)], n=4 |
| MOBA +O3→OH +HO2 +CO2 +MEK | 2E-17 |
| ETHLN +OH→CH2O +CO2 +NO2 | 1E-11 |
| PROPNN+OH →NO2 +MGLY | 1E-15 |

[1] All the “{CO2}” in this table are added to the standard chemical mechanism to achieve carbon balance in the reactions.

[2] γ is the reactive uptake coefficients used in GEOS-Chem aerosol uptake parameterization

**Table 3.** Photolysis reactions

|  |
| --- |
| O3+ hν→ OH+ OH |
| O3+ hν→ HO2+ OH |
| NO2+ hν→ NO+ O3 |
| H2O2 + hν→ OH+ OH |
| MP + hν→ CH2O+ HO2+ OH |
| CH2O + hν→ HO2+ HO2+ CO |
| CH2O+ hν→ H2+ CO |
| HNO3+ hν→ OH+ NO2 |
| HNO2+ hν→ OH+ NO |
| HNO4+ hν→ OH+ NO3 |
| NO3+ hν→ NO2+ O3 |
| NO3+ hν→ NO+ O2 |
| N2O5+ hν→ NO3+ NO2 |
| N2O5+ hν→ NO3+ NO+ O3 |
| HNO4+ hν→ HO2+ NO2 |
| ALD2+ hν→ MO2+ HO2+ CO |
| ALD2+ hν→ CH4+ CO |
| PAN+ hν→0.6MCO3+0.6NO2+0.4MO2+0.4NO3 |
| RCHO+ hν→ ETO2+ HO2+ CO |
| ACET+ hν→ MCO3+ MO2 |
| ACET+ hν→2MO2+ CO |
| MEK+ hν→ 0.85MCO3+0.85ETO2+0.15MO2+0.15RCO3 |
| GLYC+ hν→ CH2O+2HO2+ CO |
| GLYX+ hν→0.5H2+ CO+0.5CH2O+0.5CO |
| GLYX+ hν→2CO+2HO2 |
| MGLY+ hν→ MCO3+ CO+ HO2 |
| MGLY+ hν→ ALD2+ CO |
| MVK+ hν→ PRPE+ CO |
| MVK+ hν→ MCO3+ CH2O+ CO+ HO2 |
| MVK+ hν→ MO2+ MAO3 |
| MACR+ hν→ MAO3+ HO2 |
| MACR+ hν→ CO+ HO2+ CH2O+ MCO3 |
| HAC+ hν→ MCO3+ CH2O+ HO2 |
| INPN+ hν→ OH+ HO2+ RCHO+ NO2 |
| PRPN+ hν→ OH+ HO2+ RCHO+ NO2 |
| ETP+ hν→ OH+ HO2+ ALD2 |
| RA3P+ hν→ OH+ HO2+ RCHO |
| RB3P+ hν→ OH+ HO2+ ACET |
| R4P+ hν→ OH+ HO2+ RCHO |
| PP+ hν→ OH+ HO2+ ALD2+ CH2O |
| RP+ hν→ OH+ HO2+ ALD2 |
| RIP+ hν→ OH+ HO2+0.71CH2O+0.425MVK +0.285MACR+0.29HC5 |
| IAP+ hν→ OH+ HO2+0.67CO+0.19H2 +0.36HAC+0.26GLYC+0.58MGLY |
| ISNP+ hν→ OH+ HO2+ RCHO+ NO2 |
| VRP+ hν→ OH+0.3HO2+0.3CH2O+0.7MCO3 +0.7GLYC+0.3MGLY |
| MRP+ hν→ OH+ HO2+ HAC+0.5CO+0.5CH2O |
| MAOP+ hν→ OH+ CH2O+ MCO3 |
| R4N2+ hν→ NO2+0.32ACET+0.19MEK+0.18MO2+0.27HO2+0.32ALD2+0.13RCHO+0.05A3O2+0.18B3O2+0.32ETO2 |
| MAP+ hν→ OH+ MO2 |
| MACRN+ hν→ NO2+ HAC+ MGLY+0.5CH2O+ HO2+0.5CO |
| MVKN+ hν→ GLYC+ NO2+ MCO3 |
| ISOPNB+ hν→ HC5+ NO2+ HO2 |
| Br2+ hν→2Br |
| BrO+ hν→ Br+ O3 |
| HOBr+ hν→ Br+ OH |
| BrNO3+ hν→ Br+ NO3 |
| BrNO3+ hν→ BrO+ NO2 |
| BrNO2+ hν→ Br+ NO2 |
| CHBr3+ hν→2Br |
| MPN+ hν→ CH2O+ NO3+ HO2 |
| MPN+ hν→ MO2+ NO2 |
| ISOPND+ hν→ HC5+ NO2+ HO2 |
| PROPNN+ hν→ CH2O+ NO2+ CO+ MO2 |
| ATOOH+ hν→ OH+ CH2O+ MCO3 |

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