



*Supplement of*

## **Incorporating Oxygen Isotopes of Oxidized Reactive Nitrogen in the Regional Atmospheric Chemistry Mechanism, version 2 (ICOIN-RACM2)**

**Wendell W. Walters et al.**

*Correspondence to:* Wendell W. Walters (wendellw@mailbox.sc.edu)

The copyright of individual parts of the supplement might differ from the article licence.

**Table of Content:**

|  |      |
|--|------|
| <b>Table S1.</b> ICOIN-RACM2 Species .....                         | 1-5  |
| <b>Table S2.</b> ICOIN-RACM2 Photolysis Reactions .....            | 6-7  |
| <b>Table S3.</b> ICOIN-RACM2 Thermal Reactions .....               | 8-46 |
| <b>Table S4.</b> ICOIN-RACM2 Troe Reaction Parameters .....        | 47   |
| <b>Table S5.</b> ICOIN-RACM2 Troe Equilibrium Parameters .....     | 48   |
| <b>Table S6.</b> ICOIN-RACM2 Special Rate Expressions .....        | 49   |
| <b>Table S7.</b> ICOIN-RACM2(Het) Heterogeneous Reaction Additions | 50   |
| <b>References.....</b>   | 51   |

**Table S1.** ICOIN-RACM2 species list. Modified from Goliff et al., 2013 to include the addition of 55 species to track the  $\Delta^{17}\text{O}$  transfer and propagation from  $\text{O}_3$  into  $\text{NO}_y$  and  $\text{O}_x$  molecules.

| Species | Definition  | Molecular Weight |
|---------|---|------------------|
| ACD     | Acetaldehyde  | 44               |
| ACE     | Acetylene   | 26               |
| ACO3    | Acetyl peroxy radicals  | 75               |
| ACT     | Acetone   | 58               |
| ACTP    | Peroxy radicals formed from ACT                                       | 89               |
| ADCN    | Aromatic- $\text{NO}_3$ adduct from PHEN                              | 156              |
| ADCNQ   | Aromatic- $\text{NO}_3$ adduct from PHEN $\Delta^{17}\text{O}$ tracer | 156              |
| ADCNQ2  | Aromatic- $\text{NO}_3$ adduct from PHEN $\Delta^{17}\text{O}$ tracer | 156              |
| ADCNQ3  | Aromatic- $\text{NO}_3$ adduct from PHEN $\Delta^{17}\text{O}$ tracer | 156              |
| ADDc    | Aromatic-HO adduct from CSL   | 125              |
| ALD     | C3 and higher aldehydes   | 58               |
| API     | Alpha-pinenes and other cyclic terpenes with one double bond          | 136              |
| APIP    | Peroxy radicals formed from API                                       | 185              |
| BALD    | Benzaldehyde and other aromatic aldehydes                             | 106              |
| BALP    | Peroxy radicals formed from BALD                                      | 137              |
| BAL1    | Peroxy radicals formed from BALD                                      | 121              |
| BAL2    | Peroxy radicals formed from BALD                                      | 105              |
| BEN     | Benzene   | 78               |
| BENP    | Peroxy radicals formed from BEN                                       | 159              |
| CH4     | Methane   | 16               |
| CHO     | Phenoxy radical formed from CSL                                       | 139              |
| CO      | Carbon monoxide   | 28               |
| CO2     | Carbon dioxide  | 44               |
| CSL     | Cresol and other hydroxy substituted aromatics                        | 108              |
| DCB1    | Unsaturated dicarbonyls   | 91               |
| DCB2    | Unsaturated dicarbonyls   | 110              |
| DCB3    | Unsaturated dicarbonyls   | 84               |
| DIEN    | Butadiene and other anthropogenic dienes                              | 54               |
| EOH     | Ethanol   | 46               |
| EPX     | Epoxide formed in TOL, XYL and XYO reactions                          | 122              |
| ETE     | Ethene  | 28               |
| ETEG    | Ethylene glycol   | 62               |
| ETEP    | Peroxy radicals formed from ETE                                       | 77               |
| ETH     | Ethane  | 30               |
| ETHP    | Peroxy radicals formed from ETH                                       | 61               |
| GLY     | Glyoxal   | 58               |
| H2      | Hydrogen  | 2                |
| H2O     | Water   | 18               |
| H2O2    | Hydrogen peroxide   | 34               |
| H2OQ    | Hydrogen peroxide $\Delta^{17}\text{O}$ tracer                        | 34               |
| H2Q2    | Hydrogen peroxide $\Delta^{17}\text{O}$ tracer                        | 34               |

|         |  |     |
|---------|--|-----|
| HC3     | Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) less than $3.4 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$                         | 44  |
| HC3P    | Peroxy radicals formed from HC3  | 75  |
| HC5     | Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) between $3.4 \times 10^{-12}$ and $6.8 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ | 72  |
| HC5P    | Peroxy radicals formed from HC5  | 103 |
| HC8     | Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) greater than $6.8 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$                      | 114 |
| HC8P    | Peroxy radicals formed from HC8  | 145 |
| HCHO    | Formaldehyde   | 30  |
| HKET    | Hydroxy ketone   | 74  |
| HNO3    | Nitric acid  | 63  |
| HNO2Q   | Nitric acid $\Delta^{17}\text{O}$ tracer   | 63  |
| HNOQ2   | Nitric acid $\Delta^{17}\text{O}$ tracer   | 63  |
| HNQ3    | Nitric acid $\Delta^{17}\text{O}$ tracer   | 63  |
| HO2NO2  | Pernitric acid   | 79  |
| HO2NOQ  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HO2NQ2  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HOQNO2  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HOQNOQ  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HOQNOQ2 | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HQ2NO2  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HQ2NOQ  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HQ2NQ2  | Pernitric acid $\Delta^{17}\text{O}$ tracer  | 79  |
| HO      | Hydroxy radical  | 17  |
| HQ      | Hydroxy radical $\Delta^{17}\text{O}$ tracer   | 17  |
| HO2     | Hydroperoxy radical  | 33  |
| HOQ     | Hydroperoxy radical $\Delta^{17}\text{O}$ tracer   | 33  |
| HQ2     | Hydroperoxy radical $\Delta^{17}\text{O}$ tracer   | 33  |
| HONO    | Nitrous acid   | 47  |
| HONQ    | Nitrous acid $\Delta^{17}\text{O}$ tracer  | 47  |
| HQNQ    | Nitrous acid $\Delta^{17}\text{O}$ tracer  | 47  |
| ISHP    | Beta-hydroxy hydroperoxides from ISOP+HO <sub>2</sub>  | 118 |
| ISO     | Isoprene   | 68  |
| ISON    | Beta-hydroxyalkylnitrates from ISOP+NO alkylnitrates from ISO+NO <sub>3</sub>  | 147 |
| ISONQ   | Beta-hydroxyalkylnitrates from ISOP+NO alkylnitrates from ISO+NO <sub>3</sub> $\Delta^{17}\text{O}$ tracer   | 147 |
| ISONQ2  | Beta-hydroxyalkylnitrates from ISOP+NO alkylnitrates from ISO+NO <sub>3</sub> $\Delta^{17}\text{O}$ tracer   | 147 |
| ISONQ3  | Beta-hydroxyalkylnitrates from ISOP+NO alkylnitrates from ISO+NO <sub>3</sub> $\Delta^{17}\text{O}$ tracer   | 147 |
| ISOP    | Peroxy radicals formed from ISO+HO   | 117 |
| KET     | Ketones  | 86  |
| KETP    | Peroxy radicals formed from KET  | 117 |
| LIM     | d-limonene and other cyclic diene-terpenes   | 136 |
| LIMP    | Peroxy radicals formed from LIM  | 185 |

|        |  |     |
|--------|--|-----|
| MACP   | Peroxy radicals formed from MACR+HO  | 101 |
| MACR   | Methacrolein   | 70  |
| MAHP   | Hydroperoxides from MACP+HO <sub>2</sub>   | 102 |
| MCP    | Peroxy radical formed from MACR + HO which does not form MPAN  | 119 |
| MCT    | Methyl catechol  | 124 |
| MCTO   | Alkoxy radical formed from MCT+HO and MCT+NO <sub>3</sub>  | 123 |
| MCTP   | Radical formed from MCT+O <sub>3</sub> reaction  | 172 |
| MEK    | Methyl ethyl ketone  | 72  |
| MEKP   | Peroxy radicals formed from MEK  | 103 |
| MGLY   | Methylglyoxal and other alpha-carbonyl aldehydes   | 72  |
| MO2    | Methyl peroxy radical  | 47  |
| MOH    | Methanol   | 32  |
| MPAN   | Peroxymethacryloylnitrate and other higher peroxyacylnitrates from isoprene oxidation                          | 148 |
| MPANQ  | Peroxymethacryloylnitrate and other higher peroxyacylnitrates from isoprene oxidation Δ <sup>17</sup> O tracer | 148 |
| MPANQ2 | Peroxymethacryloylnitrate and other higher peroxyacylnitrates from isoprene oxidation Δ <sup>17</sup> O tracer | 148 |
| MVK    | Methyl vinyl ketone  | 70  |
| MVKP   | Peroxy radicals formed from MVK  | 119 |
| N2     | Nitrogen   | 28  |
| N2O5   | Dinitrogen pentoxide   | 108 |
| N2O4Q  | Dinitrogen pentoxide Δ <sup>17</sup> O tracer  | 108 |
| N2O3Q2 | Dinitrogen pentoxide Δ <sup>17</sup> O tracer  | 108 |
| N2O2Q3 | Dinitrogen pentoxide Δ <sup>17</sup> O tracer  | 108 |
| N2OQ4  | Dinitrogen pentoxide Δ <sup>17</sup> O tracer  | 108 |
| N2Q5   | Dinitrogen pentoxide Δ <sup>17</sup> O tracer  | 108 |
| NALD   | Nitrooxyacetaldehyde   | 105 |
| NALDQ  | Nitrooxyacetaldehyde Δ <sup>17</sup> O tracer  | 105 |
| NALDQ2 | Nitrooxyacetaldehyde Δ <sup>17</sup> O tracer  | 105 |
| NALDQ3 | Nitrooxyacetaldehyde Δ <sup>17</sup> O tracer  | 105 |
| NO     | Nitric oxide   | 30  |
| NQ     | Nitric oxide Δ <sup>17</sup> O tracer  | 30  |
| NO2    | Nitrogen dioxide   | 46  |
| NOQ    | Nitrogen dioxide Δ <sup>17</sup> O tracer  | 46  |
| NQ2    | Nitrogen dioxide Δ <sup>17</sup> O tracer  | 46  |
| NO3    | Nitrogen trioxide  | 62  |
| NO2Q   | Nitrogen trioxide Δ <sup>17</sup> O tracer   | 62  |
| NOQ2   | Nitrogen trioxide Δ <sup>17</sup> O tracer   | 62  |
| NQ3    | Nitrogen trioxide Δ <sup>17</sup> O tracer   | 62  |
| O1D    | Excited state oxygen atom, O('D)   | 16  |
| Q1D    | Excited state oxygen atom, O('D) Δ <sup>17</sup> O tracer  | 16  |
| O2     | Oxygen   | 32  |
| O3     | Ozone  | 48  |
| O3P    | Ground state oxygen atom, O( <sup>3</sup> P)   | 16  |
| Q3P    | Ground state oxygen atom, O( <sup>3</sup> P) Δ <sup>17</sup> O tracer  | 16  |

|        |  |     |
|--------|--|-----|
| OLI    | Internal alkenes   | 68  |
| OLIP   | Peroxy radicals formed from OLI  | 117 |
| OLND   | NO <sub>3</sub> -alkene adduct reacting via decomposition  | 136 |
| OLNDQ  | NO <sub>3</sub> -alkene adduct reacting via decomposition Δ <sup>17</sup> O tracer                       | 136 |
| OLNDQ2 | NO <sub>3</sub> -alkene adduct reacting via decomposition Δ <sup>17</sup> O tracer                       | 136 |
| OLNDQ3 | NO <sub>3</sub> -alkene adduct reacting via decomposition Δ <sup>17</sup> O tracer                       | 136 |
| OLNN   | NO <sub>3</sub> -alkene adduct reacting to form carbonitrates + HO <sub>2</sub>                          | 136 |
| OLNNQ  | NO <sub>3</sub> -alkene adduct reacting to form carbonitrates + HO <sub>2</sub> Δ <sup>17</sup> O tracer | 136 |
| OLNQ2  | NO <sub>3</sub> -alkene adduct reacting to form carbonitrates + HO <sub>2</sub> Δ <sup>17</sup> O tracer | 136 |
| OLNQ3  | NO <sub>3</sub> -alkene adduct reacting to form carbonitrates + HO <sub>2</sub> Δ <sup>17</sup> O tracer | 136 |
| OLT    | Terminal alkenes   | 42  |
| OLTP   | Peroxy radicals formed from OLT  | 91  |
| ONIT   | Organic nitrate  | 119 |
| ONITQ  | Organic nitrate Δ <sup>17</sup> O tracer   | 119 |
| ONITQ2 | Organic nitrate Δ <sup>17</sup> O tracer   | 119 |
| ONITQ3 | Organic nitrate Δ <sup>17</sup> O tracer   | 119 |
| OP1    | Methyl hydrogen peroxide   | 48  |
| OP2    | Higher organic peroxides   | 62  |
| ORA1   | Formic acid  | 46  |
| ORA2   | Acetic acid and higher acids   | 60  |
| ORAP   | Peroxy radical formed from ORA2 + HO reaction  | 109 |
| PAA    | Peroxyacetic acids and higher analogs  | 76  |
| PAN    | Peroxyacetyl nitrate and higher saturated PANs   | 121 |
| PANQ   | Peroxyacetyl nitrate and higher saturated PANs Δ <sup>17</sup> O tracer                                  | 121 |
| PANQ2  | Peroxyacetyl nitrate and higher saturated PANs Δ <sup>17</sup> O tracer                                  | 121 |
| PER1   | Peroxy intermediate formed from TOL  | 141 |
| PER2   | Peroxy intermediate formed from TOL  | 157 |
| PHEN   | Phenol   | 94  |
| PHO    | Phenoxy radical formed from phenol   | 93  |
| PPN    | Peroxypropionyl nitrate  | 135 |
| PPNQ   | Peroxypropionyl nitrate Δ <sup>17</sup> O tracer   | 135 |
| PPNQ2  | Peroxypropionyl nitrate Δ <sup>17</sup> O tracer   | 135 |
| RCO3   | Higher saturated acyl peroxy radicals  | 90  |
| ROH    | C3 and higher alcohols   | 60  |
| SO2    | Sulfur dioxide   | 64  |
| SULF   | Sulfuric acid  | 98  |
| TLP1   | Peroxy radicals formed from TOL  | 91  |
| TOL    | Toluene and less reactive aromatics  | 92  |
| TOLP   | Peroxy radicals formed from TOL  | 141 |
| TR2    | Peroxy radicals formed from TOL  | 109 |
| UALD   | Unsaturated aldehydes  | 84  |
| UALP   | Peroxy radicals formed from UALD   | 133 |
| XO2    | Accounts for addition NO to NO <sub>2</sub> conversions  | N/A |
| XY2    | Peroxy radicals formed from XYL  | 124 |
| XYL1   | Peroxy radicals formed from XYL  | 156 |
| XYM    | M-xylene   | 106 |

|      |                                 |     |
|------|---------------------------------|-----|
| XYP  | P-xylene                        | 106 |
| XYLP | Peroxy radicals formed from XYL | 155 |
| XYO  | o-xylene                        | 106 |
| XYO2 | Peroxy radicals formed from XYO | 155 |
| XYOP | Peroxy radicals formed from XYO | 155 |

**Table S2.** The ICOIN-RACM2 Mechanism: Photolysis Reactions.

| Reaction No. | Reaction  | Photolysis Frequency |
|--------------|---|----------------------|
| R001         | O3=Q3P+O2   | J(O3P)               |
| R002         | O3=Q1D+O2   | J(O1D)               |
| R003         | H2O2=OH+OH  | J(H2O2)              |
| R003a        | H2OQ=OH+QH  | J(H2O2)              |
| R003b        | H2Q2=QH + QH  | J(H2O2)              |
| R004         | NO2=O3P+NO  | J(NO2)               |
| R004a        | NOQ=0.5Q3P+0.5NO + 0.5O3P + 0.5NQ                                   | J(NO2)               |
| R004b        | NQ2=Q3P+NQ  | J(NO2)               |
| R005         | NO3=O2+NO   | J(NO3_NO)            |
| R005a        | NO2Q= 0.33*NQ + 0.66*NO   | J(NO3_NO)            |
| R005b        | NOQ2= 0.66*NQ + 0.33*NO   | J(NO3_NO)            |
| R005c        | NQ3=NQ  | J(NO3_NO)            |
| R006         | NO3=O3P+NO2   | J(NO3_NO2)           |
| R006a        | NO2Q=0.333*Q3P + 0.333*NO2 + 0.666*O3P + 0.666*NOQ                  | J(NO3_NO2)           |
| R006b        | NOQ2=0.666*Q3P + 0.666*NOQ + 0.333*O3P + 0.333*NQ2                  | J(NO3_NO2)           |
| R006c        | NQ3=Q3P+NQ2   | J(NO3_NO2)           |
| R007         | HONO=OH+NO  | J(HONO)              |
| R007a        | HONQ=0.5*NO +0.5*NQ + 0.5*OH + 0.5*QH                               | J(HONO)              |
| R007b        | HQNQ=QH+NQ  | J(HONO)              |
| R008         | HNO3=OH+NO2   | J(HNO3)              |
| R008a        | HNO2Q = (2/3)*NOQ + (1/3)*NO2 + (2/3)*OH + (1/3)*QH                 | J(HNO3)              |
| R008b        | HNOQ2 = (2/3)*NOQ + (1/3)*NQ2 + (2/3)*QH + (1/3)OH                  | J(HNO3)              |
| R008c        | HNQ3= NQ2 + QH  | J(HNO3)              |
| R009         | HO2NO2 = 0.2OH+0.2NO3+0.8HO2+0.8NO2                                 | J(HO2NO2)            |
| R009a        | HO2NOQ = 0.2OH+0.2NO2Q+0.8HO2+0.8NOQ                                | J(HO2NO2)            |
| R009b        | HO2NQ2 = 0.2OH+0.2NOQ2+0.8HO2+0.8NQ2                                | J(HO2NO2)            |
| R009c        | HOQNO2 =<br>0.1OH+0.1NO2Q+0.4HOQ+0.4NO2+0.1QH+0.1NO3+0.4HOQ+0.4NO2  | J(HO2NO2)            |
| R009d        | HOQNOQ =<br>0.1QH+0.1NO2Q+0.4HOQ+0.4NOQ+0.1OH+0.1NOQ2+0.4HOQ+0.4NOQ | J(HO2NO2)            |
| R009e        | HOQNQ2 =<br>0.1OH+0.1NQ3+0.4HOQ+0.4NQ2+0.1QH+0.1NOQ2+0.4HOQ+0.4NQ2  | J(HO2NO2)            |
| R009f        | HQ2NO2 = 0.2QH+0.2NO2Q+0.8HQ2+0.8NO2                                | J(HO2NO2)            |
| R009g        | HQ2NOQ = 0.2QH+0.2NOQ2+0.8HQ2+0.8NOQ                                | J(HO2NO2)            |
| R009h        | HQ2NQ2 = 0.2QH+0.2NQ3+0.8HQ2+0.8NQ2                                 | J(HO2NO2)            |
| R010         | HCHO=H2+CO  | J(HCHO_H2)           |
| R011         | HCHO=HO2+HO2+CO   | J(HCHO_HO2)          |
| R012         | ACD=HO2+MO2+CO  | J(ACD)               |
| R013         | ALD=HO2+ETHP+CO   | J(ALD)               |
| R014         | ACT=ACO3+MO2  | J(ACT)               |
| R015         | UALD=1.22HO2+0.784ACO3+1.22CO+0.35HCHO+0.434ALD+0.216KET            | J(UALD)              |
| R016         | MEK=ACO3+0.5ETHP+0.5MO2   | J(MEK)               |

|       |   |         |
|-------|---|---------|
| R017  | KET=ETHP+ACO3   | J(KET)  |
| R018  | HKET=HO2+ACO3+HCHO  | J(HKET) |
| R019  | MACR=0.34OH+0.66HO2+0.67ACO3+0.33MACP+0.34XO2+0.67CO+0.67HCHO | J(MACR) |
| R020  | MVK=0.7UALD+0.7CO+0.3MO2+0.3MACP                              | J(MVK)  |
| R021  | GLY=H2+CO+CO  | J(GLY1) |
| R022  | GLY=HCHO+CO+CO  | J(GLY2) |
| R023  | GLY=HO2+HO2+CO+CO   | J(GLY3) |
| R024  | MGLY=HO2+ACO3+CO  | J(MGLY) |
| R025  | DCB1=2XO2+1.5HO2+0.5GLY+0.5MGLY+CO+0.5ACO3                    | J(DCB1) |
| R026  | DCB2=2XO2+1.5HO2+0.5GLY+0.5MGLY+CO+0.5ACO3                    | J(DCB2) |
| R027  | BALD=CHO+HO2+CO   | J(BALD) |
| R028  | OP1=OH+HO2+HCHO   | J(OP1)  |
| R029  | OP2=OH+HO2+ALD  | J(OP2)  |
| R030  | PAA=OH+MO2  | J(PAA)  |
| R031  | ONIT=HO2+0.2ALD+NO2+0.8KET                                    | J(ONIT) |
| R031a | ONITQ=HO2+0.2ALD+(2/3)*NOQ+(1/3)*NO2+0.8KET                   | J(ONIT) |
| R031b | ONITQ2=HO2+0.2ALD+(2/3)*NOQ+(1/3)*NQ2+0.8KET                  | J(ONIT) |
| R031c | ONITQ3=HOQ+0.2ALD+NQ2+0.8KET                                  | J(ONIT) |
| R032  | PAN=ACO3+NO2  | J(PAN1) |
| R032a | PANQ=ACO3+NOQ   | J(PAN1) |
| R032b | PANQ2=ACO3+NQ2  | J(PAN1) |
| R033  | PAN=MO2+NO3+CO2   | J(PAN2) |
| R033a | PANQ=MO2+NO2Q+CO2   | J(PAN2) |
| R033b | PANQ2=MO2+NOQ2+CO2  | J(PAN2) |

<sup>a</sup>The photolysis frequency ( $J$ ) were calculated in the F0AM model using literature derived cross sections and quantum yields taken from latest IUPAC and JPL recommendations as previously documented (Wolfe et al., 2016).

**Table S3.** The ICOIN-RACM2 Mechanism: Thermal Reactions.

| Reaction No.               | Reaction  | Reaction Rate                                  | Note |
|----------------------------|---|--|------|
| <b>Inorganic Reactions</b> |   |  |      |
| R034                       | O <sub>3</sub> +OH=HOQ+O <sub>2</sub>   | 1.70E-12.*exp(-940./T)                         | 1    |
| R034a                      | O <sub>3</sub> +QH=HQ2+O <sub>2</sub>   | 1.70E-12.*exp(-940./T)                         | 1    |
| R035                       | O <sub>3</sub> +HO <sub>2</sub> =OH+O <sub>2</sub> +O <sub>2</sub>                | 1.00E-14.*exp(-490./T)                         | 1    |
| R035a                      | O <sub>3</sub> +HOQ=0.5QH+0.5OH   | 1.00E-14.*exp(-490./T)                         | 1    |
| R035b                      | O <sub>3</sub> +HQ2=QH  | 1.00E-14.*exp(-490./T)                         | 1    |
| R036                       | O <sub>3</sub> +NO=NOQ+O <sub>2</sub>   | 1.40e-12.*exp(-1310./T)                        | 1    |
| R036a                      | O <sub>3</sub> +NQ=NQ2+O <sub>2</sub>   | 1.40e-12.*exp(-1310./T)                        | 1    |
| R037                       | NO <sub>2</sub> +O <sub>3</sub> =NO2Q+O <sub>2</sub>                              | 1.40e-13.*exp(-2470./T)                        | 1    |
| R037a                      | NOQ+O <sub>3</sub> =NOQ2+O <sub>2</sub>   | 1.40e-13.*exp(-2470./T)                        | 1    |
| R037b                      | NQ2+O <sub>3</sub> =NQ3+O <sub>2</sub>  | 1.40e-13.*exp(-2470./T)                        | 1    |
| R038                       | O <sub>3</sub> P+O <sub>2</sub> =O <sub>3</sub>                                   | M.*5.60E-34.*((T./300).^-2.6).*0.21.*M         | 1    |
| R038a                      | Q3P+O <sub>2</sub> =O <sub>3</sub>  | M.*5.60E-34.*((T./300).^-2.6).*0.21.*M         | 1    |
| R039                       | O <sub>3</sub> P+O <sub>3</sub> =O <sub>2</sub> +O <sub>2</sub>                   | 8.00e-12.*exp(-2060./T)                        | 1    |
| R039a                      | Q3P+O <sub>3</sub> =O <sub>2</sub> +O <sub>2</sub>                                | 8.00e-12.*exp(-2060./T)                        | 1    |
| R040                       | O1D+O <sub>2</sub> =O3P+O <sub>2</sub>  | 3.20e-11.*0.21.*M                              | 1    |
| R040a                      | Q1D+O <sub>2</sub> =Q3P   | 3.20e-11.*0.21.*M                              | 1    |
| R041                       | O1D+N2=O3P+N2   | 1.80e-11.*exp(107./T).*0.78.*M                 | 1    |
| R041a                      | Q1D+N2=Q3P+N2   | 1.80e-11.*exp(107./T).*0.78.*M                 | 1    |
| R042                       | O1D+H <sub>2</sub> O=OH+OH  | 2.20E-10.*H <sub>2</sub> O                     | 1    |
| R042a                      | Q1D+H <sub>2</sub> O=QH+OH  | 2.20E-10.*H <sub>2</sub> O                     | 1    |
| R043                       | OH+H <sub>2</sub> =HO <sub>2</sub> +H <sub>2</sub> O                              | 7.70e-12.*exp(-2100./T)                        | 1    |
| R043a                      | QH+H <sub>2</sub> =HO <sub>2</sub> +H <sub>2</sub> O                              | 7.70e-12.*exp(-2100./T)                        | 1    |
| R044                       | OH+HO <sub>2</sub> =H <sub>2</sub> O+O <sub>2</sub>                               | 4.80E-11.*exp(250./T)                          | 1    |
| R044a                      | QH+HO <sub>2</sub> =H <sub>2</sub> O+O <sub>2</sub>                               | 4.80E-11.*exp(250./T)                          | 1    |
| R044b                      | QH+HOQ= H <sub>2</sub> O+O <sub>2</sub>   | 4.80E-11.*exp(250./T)                          | 1    |
| R044c                      | QH+HQ2= H <sub>2</sub> O+O <sub>2</sub>   | 4.80E-11.*exp(250./T)                          | 1    |
| R044d                      | OH+HQ2= H <sub>2</sub> O+O <sub>2</sub>   | 4.80E-11.*exp(250./T)                          | 1    |
| R044e                      | OH+HOQ= H <sub>2</sub> O+O <sub>2</sub>   | 4.80E-11.*exp(250./T)                          | 1    |
| R045                       | HO <sub>2</sub> +HO <sub>2</sub> =H <sub>2</sub> O <sub>2</sub> +O <sub>2</sub>   | 2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T) | 1    |
| R045a                      | HOQ + HO <sub>2</sub> = 0.5*H <sub>2</sub> OQ + 0.5*H <sub>2</sub> O <sub>2</sub> | 2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T) | 1    |

|       |  |  |         |
|-------|--|--|---------|
| R045b | $HQ_2 + HO_2 = H_2OQ$                                  | $2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T)$           | 1       |
| R045c | $HOQ + HOQ = 0.25*H_2O_2 + 0.5*H_2OQ + 0.25*HQ_2$      | $2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T)$           | 1       |
| R045d | $HQ_2 + HOQ = 0.5*H_2OQ + 0.5*HQ_2$                    | $2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T)$           | 1       |
| R045e | $HQ_2 + HQ_2 = H_2Q_2$                                 | $2.20e-13.*exp(600./T)+1.90e-33.*M.*exp(980./T)$           | 1       |
| R046  | $HO_2+HO_2+H_2O=H_2O_2+H_2O+O_2$                       | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R046a | $HOQ + HO_2 = 0.5*H_2OQ + 0.5*H_2O_2+O_2$              | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R046b | $HQ_2 + HO_2 = H_2OQ +O_2$                             | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R046c | $HOQ + HOQ = 0.5*H_2OQ + 0.25*HQ_2 + 0.25*H_2O_2 +O_2$ | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R046d | $HOQ + HQ_2 = 0.5*HQ_2 + 0.5*H_2OQ +O_2$               | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R046e | $HQ_2 + HQ_2 = H_2Q_2 +O_2$                            | $(3.08e-34.*exp(2800./T)+2.59e-54.*M.*exp(3180./T)).*H_2O$ | 1       |
| R047  | $H_2O_2+OH=HO_2+H_2O$                                  | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R047a | $H_2OQ+OH=0.5HOQ+0.5HO_2 +H_2O$                        | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R047b | $HQ_2+OH=HOQ+H_2O$                                     | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R047c | $H_2O_2+QH=HOQ+H_2O$                                   | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R047d | $H_2OQ+QH=0.5HQ_2+0.5HOQ+H_2O$                         | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R047e | $HQ_2+QH=HQ_2+H_2O$                                    | $2.90E-12.*exp(-160./T)$                                   | 1       |
| R048  | $NO+O_3P=NO_2$   | $K_O3P_NO$   | Table 4 |
| R048a | $NQ+O_3P=NOQ$  | $K_O3P_NO$   | Table 4 |
| R048b | $NQ+Q_3P=NQ_2$   | $K_O3P_NO$   | Table 4 |
| R048c | $NO+Q_3P=NOQ$  | $K_O3P_NO$   | Table 4 |
| R049  | $NO+OH=HONO$   | $K_OH_NO$  | 1       |

|       |  |                              |         |
|-------|--|------------------------------|---------|
| R049a | NQ+OH=HONQ                                 | K_OH_NO                      | 1       |
| R049b | NQ+QH=HQNQ                                 | K_OH_NO                      | 1       |
| R049c | NO+QH=HONQ                                 | K_OH_NO                      | 1       |
| R050  | HO2+NO=OH+NO2                              | 3.45E-12.*exp(270./T)        | 1       |
| R050a | HO2+NQ=OH+NOQ                              | 3.45E-12.*exp(270./T)        | 1       |
| R050b | HOQ+NQ=0.5*QH + 0.5*NOQ + 0.5*OH + 0.5*NQ2 | 3.45E-12.*exp(270./T)        | 1       |
| R050c | HQ2+NQ=QH+NQ2                              | 3.45E-12.*exp(270./T)        | 1       |
| R050d | HOQ+NO=0.5OH+0.5NOQ+0.5QH+0.5NO2           | 3.45E-12.*exp(270./T)        | 1       |
| R050e | HQ2+NO=QH+NOQ                              | 3.45E-12.*exp(270./T)        | 1       |
| R051  | HO2+NO=HNO3                                | K_HO2_NO_HNO3                | Table 6 |
| R051a | HO2+NQ=HNO2Q                               | K_HO2_NO_HNO3                | Table 6 |
| R051b | HOQ+NQ=HNOQ2                               | K_HO2_NO_HNO3                | Table 6 |
| R051c | HQ2+NQ=HNQ3                                | K_HO2_NO_HNO3                | Table 6 |
| R051d | HQ2+NO=HNOQ2                               | K_HO2_NO_HNO3                | Table 6 |
| R051e | HOQ+NO=HNO2Q                               | K_HO2_NO_HNO3                | Table 6 |
| R052  | NO+NO+O2=NO2+NO2                           | 3.30e-39.*exp(530./T).*21.*M | 1       |
| R052a | NQ+NO+O2=NOQ+NO2                           | 3.30e-39.*exp(530./T).*21.*M | 1       |
| R052b | NQ+NQ+O2=NOQ+NOQ                           | 3.30e-39.*exp(530./T).*21.*M | 1       |
| R053  | HONO+OH=NO2+H2O                            | 2.50e-12.*exp(260./T)        | 1       |
| R053a | HONO+QH=NO2                                | 2.50e-12.*exp(260./T)        | 1       |
| R053b | HONQ+QH=NOQ                                | 2.50e-12.*exp(260./T)        | 1       |
| R053c | HQNQ+QH=NQ2                                | 2.50e-12.*exp(260./T)        | 1       |
| R053d | HQNQ+OH=NQ2                                | 2.50e-12.*exp(260./T)        | 1       |
| R053e | HONQ+OH=NOQ                                | 2.50e-12.*exp(260./T)        | 1       |
| R054  | O3P+NO2=NO+O2                              | 5.50e-12.*exp(188./T)        | 1       |
| R054a | Q3P+NO2=NO+O2                              | 5.50e-12.*exp(188./T)        | 1       |
| R054b | Q3P+NOQ=0.5NQ + 0.5NO+O2                   | 5.50e-12.*exp(188./T)        | 1       |
| R054c | O3P+NOQ=NO+QO NQ+O2                        | 5.50e-12.*exp(188./T)        | 1       |
| R054d | O3P+NQ2=NQ+O2                              | 5.50e-12.*exp(188./T)        | 1       |
| R054e | Q3P+NQ2=NQ+O2                              | 5.50e-12.*exp(188./T)        | 1       |
| R055  | O3P+NO2=NO3                                | K_O3P_NO2                    | Table 4 |
| R055a | Q3P+NO2=NO2Q                               | K_O3P_NO2                    | Table 4 |
| R055b | Q3P+NOQ=NOQ2                               | K_O3P_NO2                    | Table 4 |
| R055c | Q3P+NQ2=NQ3                                | K_O3P_NO2                    | Table 4 |
| R055d | O3P+NQ2=NOQ2                               | K_O3P_NO2                    | Table 4 |
| R055e | O3P+NOQ=NO2Q                               | K_O3P_NO2                    | Table 4 |
| R056  | OH+NO2=HNO3                                | K_OH_NO2_HONO2               | Table 4 |
| R056a | QH+NO2=HNO2Q                               | K_OH_NO2_HONO2               | Table 4 |
| R056b | QH+NOQ=HNOQ2                               | K_OH_NO2_HONO2               | Table 4 |
| R056c | QH+NQ2=HNQ3                                | K_OH_NO2_HONO2               | Table 4 |
| R056d | OH+NQ2=HNOQ2                               | K_OH_NO2_HONO2               | Table 4 |

|       |   |                       |         |
|-------|---|-----------------------|---------|
| R056e | $\text{OH} + \text{NOQ} = \text{HNO}_2\text{Q}$   | K_OH_NO2_HONO2        | Table 4 |
| R057  | $\text{OH} + \text{HNO}_3 = \text{NO}_3 + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057a | $\text{QH} + \text{HNO}_3 = \text{NO}_3 + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057b | $\text{QH} + \text{HNO}_2\text{Q} = \text{NO}_2\text{Q} + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057c | $\text{QH} + \text{HNO}_2\text{Q} = \text{NO}_2\text{Q} + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057d | $\text{QH} + \text{HNQ}_3 = \text{NQ}_3 + \text{H}_2\text{Q}$   | K_OH_HNO3             | Table 6 |
| R057e | $\text{OH} + \text{HNQ}_3 = \text{NQ}_3 + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057f | $\text{OH} + \text{HNO}_2\text{Q} = \text{NO}_2\text{Q} + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R057g | $\text{OH} + \text{HNO}_2\text{Q} = \text{NO}_2\text{Q} + \text{H}_2\text{O}$   | K_OH_HNO3             | Table 6 |
| R058  | $\text{OH} + \text{NO}_3 = \text{HO}_2 + \text{NO}_2$   | 2.00e-11              | 1       |
| R058a | $\text{QH} + \text{NO}_3 = \text{HOQ} + \text{NO}_2$  | 2.00e-11              | 1       |
| R058b | $\text{QH} + \text{NO}_2\text{Q} = 0.5\text{HQ}_2 + 0.5\text{NO}_2 + 0.5\text{HOQ} + 0.5\text{NOQ}$                               | 2.00e-11              | 1       |
| R058c | $\text{QH} + \text{NO}_2\text{Q} = 0.5\text{HQ}_2 + 0.5\text{NOQ} + 0.5\text{HOQ} + 0.5\text{NQ}_2$                               | 2.00e-11              | 1       |
| R058d | $\text{QH} + \text{NQ}_3 = \text{HQ}_2 + \text{NQ}_2$   | 2.00e-11              | 1       |
| R058e | $\text{OH} + \text{NQ}_3 = \text{HOQ} + \text{NQ}_2$  | 2.00e-11              | 1       |
| R058f | $\text{OH} + \text{NO}_2\text{Q} = 0.5\text{HO}_2 + 0.5\text{NQ}_2 + 0.5\text{HOQ} + 0.5\text{NOQ}$                               | 2.00e-11              | 1       |
| R058g | $\text{OH} + \text{NO}_2\text{Q} = 0.5\text{HOQ} + 0.5\text{NO}_2 + 0.5\text{HO}_2 + 0.5\text{NOQ}$                               | 2.00e-11              | 1       |
| R059  | $\text{HO}_2 + \text{NO}_3 = 0.7\text{OH} + 0.7\text{NO}_2 + 0.3\text{HNO}_3$   | 4.00e-12              | 1       |
| R059a | $\text{HOQ} + \text{NO}_3 = 0.35\text{OH} + 0.35\text{QH} + 0.3\text{HNO}_3 + 0.7\text{NO}_2$                                     | 4.00e-12              | 1       |
| R059b | $\text{HQ}_2 + \text{NO}_3 = 0.7\text{QH} + 0.7\text{NO}_2 + 0.3\text{HNO}_3$   | 4.00e-12              | 1       |
| R059c | $\text{HQ}_2 + \text{NO}_2\text{Q} = 0.7\text{QH} + 0.3\text{HNO}_3 + 0.467\text{NQ}_2 + 0.233\text{NO}_2$                        | 4.00e-12              | 1       |
| R059d | $\text{HQ}_2 + \text{NO}_2\text{Q} = 0.7\text{QH} + 0.3\text{HNO}_2\text{Q} + 0.467\text{NOQ} + 0.233\text{NQ}_2$                 | 4.00e-12              | 1       |
| R059e | $\text{HQ}_2 + \text{NQ}_3 = 0.7\text{QH} + 0.7\text{NQ}_2 + 0.3\text{HNQ}_3$   | 4.00e-12              | 1       |
| R059f | $\text{HOQ} + \text{NQ}_3 = 0.35\text{OH} + 0.35\text{QH} + 0.3\text{HNQ}_3 + 0.7\text{NQ}_2$                                     | 4.00e-12              | 1       |
| R059g | $\text{HOQ} + \text{NO}_2\text{Q} = 0.35\text{OH} + 0.35\text{QH} + 0.3\text{HNO}_2\text{Q} + 0.467\text{NOQ} + 0.233\text{NQ}_2$ | 4.00e-12              | 1       |
| R059h | $\text{HOQ} + \text{NO}_2\text{Q} = 0.35\text{OH} + 0.35\text{QH} + 0.3\text{HNO}_2\text{Q} + 0.467\text{NOQ} + 0.233\text{NO}_2$ | 4.00e-12              | 1       |
| R059i | $\text{HO}_2 + \text{NO}_2\text{Q} = 0.7\text{OH} + 0.3\text{HNO}_2\text{Q} + 0.467\text{NOQ} + 0.233\text{NO}_2$                 | 4.00e-12              | 1       |
| R059j | $\text{HO}_2 + \text{NO}_2\text{Q} = 0.7\text{OH} + 0.3\text{HNO}_2\text{Q} + 0.467\text{NOQ} + 0.233\text{NQ}_2$                 | 4.00e-12              | 1       |
| R059k | $\text{HO}_2 + \text{NQ}_3 = 0.7\text{OH} + 0.3\text{HNQ}_3 + 0.7\text{NQ}_2$   | 4.00e-12              | 1       |
| R060  | $\text{NO} + \text{NO}_3 = \text{NO}_2 + \text{NO}_2$   | 1.80E-11.*exp(110./T) | 1       |
| R060a | $\text{NQ} + \text{NO}_3 = \text{NOQ} + \text{NO}_2$  | 1.80E-11.*exp(110./T) | 1       |
| R060b | $\text{NQ} + \text{NO}_2\text{Q} = 0.333\text{NQ}_2 + 0.333\text{NO}_2 + 1.333\text{NOQ}$   | 1.80E-11.*exp(110./T) | 1       |
| R060c | $\text{NQ} + \text{NO}_2\text{Q} = \text{NOQ} + \text{NQ}_2$  | 1.80E-11.*exp(110./T) | 1       |

|       |   |                         |         |
|-------|---|-------------------------|---------|
| R060d | $NQ + NQ_3 = 2*NQ_2$                                    | 1.80E-11.*exp(110./T)   | 1       |
| R060e | $NO + NO_2Q = NO_2 + NOQ$                               | 1.80E-11.*exp(110./T)   | 1       |
| R060f | $NO + NO_2Q = 1.333*NOQ + 0.333*NO_2 + 0.333*NQ_2$      | 1.80E-11.*exp(110./T)   | 1       |
| R060g | $NO + NQ_3 = NOQ + NQ_2$                                | 1.80E-11.*exp(110./T)   | 1       |
| R061  | $NO_2+NO_3=NO+NO_2+O_2$                                 | 4.50e-14.*exp(-1260./T) | 1       |
| R061a | $NOQ+NO_3=0.5NO+0.5NQ+NO_2$                             | 4.50e-14.*exp(-1260./T) | 1       |
| R061b | $NQ_2+NO_3=NQ+NQ_2$                                     | 4.50e-14.*exp(-1260./T) | 1       |
| R061c | $NQ_2+NO_2Q=NQ+0.33NO_2+0.66NOQ$                        | 4.50e-14.*exp(-1260./T) | 1       |
| R061d | $NQ_2+NOQ_2=NQ+0.33NQ_2+0.66NOQ$                        | 4.50e-14.*exp(-1260./T) | 1       |
| R061e | $NQ_2+NQ_3=NQ+NQ_2$                                     | 4.50e-14.*exp(-1260./T) | 1       |
| R061f | $NOQ+NQ_3=0.5NO+0.5NQ+NQ_2$                             | 4.50e-14.*exp(-1260./T) | 1       |
| R061g | $NOQ+NOQ_2=0.5NO+0.5NQ+0.66NOQ+0.333NQ_2$               | 4.50e-14.*exp(-1260./T) | 1       |
| R061h | $NOQ+NO_2Q=0.5NO+0.5NQ+0.66NOQ+0.33NO_2$                | 4.50e-14.*exp(-1260./T) | 1       |
| R061i | $NO_2+NO_2Q=NO+0.33NO_2+0.66NOQ$                        | 4.50e-14.*exp(-1260./T) | 1       |
| R061j | $NO_2+NOQ_2=NO+0.33NQ_2+0.66NOQ$                        | 4.50e-14.*exp(-1260./T) | 1       |
| R061k | $NO_2+NQ_3=NO+NQ_2$                                     | 4.50e-14.*exp(-1260./T) | 1       |
| R062  | $NO_3+NO_3=NO_2+NO_2+O_2$                               | 8.50E-13.*exp(-2450./T) | 1       |
| R062a | $NO_2Q + NO_3 = (2/3)*NOQ + (4/3)*NO_2+O_2$             | 8.50E-13.*exp(-2450./T) | 1       |
| R062b | $NOQ_2 + NO_3 = (2/3)*NOQ + (1/3)*NQ_2 + NO_2+O_2$      | 8.50E-13.*exp(-2450./T) | 1       |
| R062c | $NQ_3 + NO_3 = NQ_2 + NO_2+O_2$                         | 8.50E-13.*exp(-2450./T) | 1       |
| R062d | $NQ_3 + NO_2Q = NQ_2 + (2/3)*NOQ + (1/3)*NO_2+O_2$      | 8.50E-13.*exp(-2450./T) | 1       |
| R062e | $NQ_3 + NQ_3 = NQ_2 + NQ_2+O_2$                         | 8.50E-13.*exp(-2450./T) | 1       |
| R062f | $NO_2Q + NO_2Q = (4/3)*NOQ + (2/3)*NO_2+O_2$            | 8.50E-13.*exp(-2450./T) | 1       |
| R062g | $NO_2Q + NOQ_2 = (4/3)*NOQ (1/3)*NO_2 + (1/3)*NQ_2+O_2$ | 8.50E-13.*exp(-2450./T) | 1       |
| R062h | $NOQ_2 + NOQ_2 = (4/3)*NOQ + (2/3)*NQ_2+O_2$            | 8.50E-13.*exp(-2450./T) | 1       |
| R062i | $NOQ_2 + NQ_3 = (2/3)*NOQ + (4/3)*NQ_2+O_2$             | 8.50E-13.*exp(-2450./T) | 1       |
| R063  | $NO_2+NO_3=N2O5$  | K_NO2_NO3               | Table 4 |
| R063a | $NOQ+NO_3=N2O4Q$  | K_NO2_NO3               | Table 4 |
| R063b | $NQ_2+NO_3=N2O3Q2$                                      | K_NO2_NO3               | Table 4 |
| R063c | $NQ_2+NO_2Q=N2O2Q3$                                     | K_NO2_NO3               | Table 4 |
| R063d | $NQ_2+NOQ_2=N2OQ4$                                      | K_NO2_NO3               | Table 4 |
| R063e | $NQ_2+NQ_3=N2Q5$  | K_NO2_NO3               | Table 4 |
| R063f | $NOQ+NQ_3=N2OQ4$  | K_NO2_NO3               | Table 4 |
| R063g | $NOQ+NOQ_2=N2O2Q3$                                      | K_NO2_NO3               | Table 4 |
| R063h | $NOQ+NO_2Q=N2O3Q2$                                      | K_NO2_NO3               | Table 4 |
| R063i | $NO_2+NO_2Q=N2O4Q$                                      | K_NO2_NO3               | Table 4 |

|       |   |                       |         |
|-------|---|-----------------------|---------|
| R063j | $\text{NO}_2 + \text{NOQ}_2 = \text{N}_2\text{O}_3\text{Q}_2$   | K_NO2_NO3             | Table 4 |
| R063k | $\text{NO}_2 + \text{NQ}_3 = \text{N}_2\text{O}_2\text{Q}_3$  | K_NO2_NO3             | Table 4 |
| R064  | $\text{N}_2\text{O}_5 = \text{NO}_2 + \text{NO}_3$  | K_N2O5                | Table 5 |
| R064a | $\text{N}_2\text{O}_4\text{Q} = (2/5)*\text{NOQ} + (2/5)*\text{NO}_3 + (3/5)*\text{NO}_2 + (3/5)*\text{NO}_2\text{Q}$   | K_N2O5                | Table 5 |
| R064b | $\text{N}_2\text{O}_3\text{Q}_2 = 0.3*\text{NO}_2 + 0.6*\text{NOQ} + 0.1*\text{NQ}_2 + 0.1*\text{NO}_3 + 0.6*\text{NO}_2\text{Q} + 0.3*\text{NOQ}_2$                                      | K_N2O5                | Table 5 |
| R064c | $\text{N}_2\text{O}_2\text{Q}_3 = 0.1*\text{NO}_2 + 0.6*\text{NOQ} + 0.3*\text{NQ}_2 + 0.3*\text{NO}_2\text{Q} + 0.6*\text{NOQ}_2 + 0.1*\text{NQ}_3$                                      | K_N2O5                | Table 5 |
| R064d | $\text{N}_2\text{OQ}_4 = 0.4*\text{NOQ} + 0.6*\text{NQ}_2 + 0.6*\text{NOQ}_2 + 0.4*\text{NQ}_3$   | K_N2O5                | Table 5 |
| R064e | $\text{N}_2\text{Q}_5 = \text{NQ}_3 + \text{NQ}_2$  | K_N2O5                | Table 5 |
| R065  | $\text{N}_2\text{O}_5 + \text{H}_2\text{O} = \text{HNO}_3 + \text{HNO}_3$   | 2.50E-22.*H2O         | 1       |
| R065a | $\text{N}_2\text{O}_4\text{Q} + \text{H}_2\text{O} = (2/5)*\text{HNO}_2\text{Q} + (2/5)*\text{HNO}_3 + (3/5)*\text{HNO}_3 + (3/5)*\text{HNO}_2\text{Q}$                                   | 2.50E-22.*H2O         | 1       |
| R065b | $\text{N}_2\text{O}_3\text{Q}_2 + \text{H}_2\text{O} = 0.3*\text{HNO}_3 + 0.6*\text{HNO}_2\text{Q} + 0.1*\text{HNOQ}_2 + 0.1*\text{HNO}_3 + 0.6*\text{HNO}_2\text{Q} + 0.3*\text{HNOQ}_2$ | 2.50E-22.*H2O         | 1       |
| R065c | $\text{N}_2\text{O}_2\text{Q}_3 + \text{H}_2\text{O} = 0.1*\text{HNO}_3 + 0.6*\text{HNO}_2\text{Q} + 0.3*\text{HNOQ}_2 + 0.3*\text{HNO}_2\text{Q} + 0.6*\text{HNOQ}_2 + 0.1*\text{HNQ}_3$ | 2.50E-22.*H2O         | 1       |
| R065d | $\text{N}_2\text{OQ}_4 + \text{H}_2\text{O} = 0.4*\text{HNO}_2\text{Q} + 0.6*\text{HNOQ}_2 + 0.6*\text{HNOQ}_2 + 0.4*\text{HNQ}_3$  | 2.50E-22.*H2O         | 1       |
| R065e | $\text{N}_2\text{Q}_5 + \text{H}_2\text{O} = \text{HNQ}_3 + \text{HNOQ}_2$  | 2.50E-22.*H2O         | 1       |
| R066  | $\text{HO}_2 + \text{NO}_2 = \text{HO}_2\text{NO}_2$  | K_HO2_NO2             | Table 4 |
| R066a | $\text{HOQ} + \text{NO}_2 = \text{HOQNO}_2$   | K_HO2_NO2             | Table 4 |
| R066b | $\text{HQ}_2 + \text{NO}_2 = \text{HQ}_2\text{NO}_2$  | K_HO2_NO2             | Table 4 |
| R066c | $\text{HQ}_2 + \text{NQ}_2 = \text{HQ}_2\text{NQ}_2$  | K_HO2_NO2             | Table 4 |
| R066d | $\text{HQ}_2 + \text{NOQ} = \text{HQ}_2\text{NOQ}$  | K_HO2_NO2             | Table 4 |
| R066e | $\text{HOQ} + \text{NOQ} = \text{HOQNOQ}$   | K_HO2_NO2             | Table 4 |
| R066f | $\text{HOQ} + \text{NQ}_2 = \text{HOQNQ}_2$   | K_HO2_NO2             | Table 4 |
| R066g | $\text{HO}_2 + \text{NQ}_2 = \text{HO}_2\text{NQ}_2$  | K_HO2_NO2             | Table 4 |
| R066h | $\text{HO}_2 + \text{NOQ} = \text{HO}_2\text{NOQ}$  | K_HO2_NO2             | Table 4 |
| R067  | $\text{HO}_2\text{NO}_2 = \text{HO}_2 + \text{NO}_2$  | K_HO2NO2              | Table 5 |
| R067a | $\text{HOQNO}_2 = \text{HOQ} + \text{NO}_2$   | K_HO2NO2              | Table 5 |
| R067b | $\text{HQ}_2\text{NO}_2 = \text{HQ}_2 + \text{NO}_2$  | K_HO2NO2              | Table 5 |
| R067c | $\text{HQ}_2\text{NOQ} = \text{HQ}_2 + \text{NOQ}$  | K_HO2NO2              | Table 5 |
| R067d | $\text{HQ}_2\text{NQ}_2 = \text{HQ}_2 + \text{NQ}_2$  | K_HO2NO2              | Table 5 |
| R067e | $\text{HOQNQ}_2 = \text{HOQ} + \text{NQ}_2$   | K_HO2NO2              | Table 5 |
| R067f | $\text{HOQNOQ} = \text{HOQ} + \text{NOQ}$   | K_HO2NO2              | Table 5 |
| R067g | $\text{HO}_2\text{NOQ} = \text{HO}_2 + \text{NOQ}$  | K_HO2NO2              | Table 5 |
| R067h | $\text{HO}_2\text{NQ}_2 = \text{HO}_2 + \text{NQ}_2$  | K_HO2NO2              | Table 5 |
| R068  | $\text{OH} + \text{HO}_2\text{NO}_2 = \text{NO}_2 + \text{H}_2\text{O} + \text{O}_2$  | 1.30e-12.*exp(380./T) | 1       |

|                 |  |                                 |         |
|-----------------|--|---------------------------------|---------|
| R068a           | $QH + HO_2NO_2 = NO_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068b           | $QH + HOQNQ_2 = NO_2 + H_2Q + O_2$                                 | $1.30e-12.*exp(380./T)$         | 1       |
| R068c           | $QH + HQ_2NO_2 = NO_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068d           | $QH + HQ_2NOQ = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R068e           | $QH + HQ_2NQ_2 = NQ_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068f           | $QH + HOQNQ_2 = NQ_2 + H_2Q + O_2$                                 | $1.30e-12.*exp(380./T)$         | 1       |
| R068g           | $QH + HOQNQ_2 = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R068h           | $QH + HO_2NQ_2 = NQ_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068i           | $QH + HO_2NOQ = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R068j           | $OH + HOQNQ_2 = NO_2 + H_2O + O_2$                                 | $1.30e-12.*exp(380./T)$         | 1       |
| R068k           | $OH + HQ_2NO_2 = NO_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068l           | $OH + HQ_2NOQ = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R068m           | $OH + HQ_2NQ_2 = NQ_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068n           | $OH + HOQNQ_2 = NQ_2 + H_2Q + O_2$                                 | $1.30e-12.*exp(380./T)$         | 1       |
| R068o           | $OH + HOQNQ_2 = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R068p           | $OH + HO_2NQ_2 = NQ_2 + H_2Q + O_2$                                | $1.30e-12.*exp(380./T)$         | 1       |
| R068q           | $OH + HO_2NOQ = NOQ + H_2Q + O_2$                                  | $1.30e-12.*exp(380./T)$         | 1       |
| R069            | $OH + SO_2 = HO_2 + SULF$  | K_OH_SO2                        | Table 4 |
| R069a           | $QH + SO_2 = HO_2 + SULF$  | K_OH_SO2                        | Table 4 |
| R070            | $OH + CO = HO_2 + CO_2$  | K_OH_CO                         | Table 6 |
| R070a           | $QH + CO = HO_2 + CO_2$  | K_OH_CO                         | Table 6 |
| <b>VOC + OH</b> |  |                                 |         |
| R071            | $OH + CH_4 = MO_2 + H_2O$  | $1.85e-12.*exp(-1690./T)$       | 1       |
| R071a           | $QH + CH_4 = MO_2 + H_2O$  | $1.85e-12.*exp(-1690./T)$       | 1       |
| R072            | $ETH + OH = ETP + H_2O$  | $6.90E-12.*exp(-1000./T)$       | 1       |
| R072a           | $ETH + QH = ETP + H_2O$  | $6.90E-12.*exp(-1000./T)$       | 1       |
| R073            | $OH + HC_3 = HC_3P + H_2O$   | $7.68e-12.*exp(-370./T)$        | 1       |
| R073a           | $QH + HC_3 = HC_3P + H_2O$   | $7.68e-12.*exp(-370./T)$        | 1       |
| R074            | $OH + HC_5 = HC_5P + H_2O$   | $1.01e-11.*exp(-245./T)$        | 1       |
| R074a           | $QH + HC_5 = HC_5P + H_2O$   | $1.01e-11.*exp(-245./T)$        | 1       |
| R075            | $OH + HC_8 = 0.049HO_2 + 0.951HC_8P + H_2O$<br>+0.025ALD+0.024HKET | $2.82e-11.*exp(-273./T).*0.951$ | 1       |
| R075a           | $QH + HC_8 = 0.049HO_2 + 0.951HC_8P + H_2O$<br>+0.025ALD+0.024HKET | $2.82e-11.*exp(-273./T).*0.951$ | 1       |
| R076            | $ETE + OH = ETEP$  | K_OH_ETE                        | Table 4 |
| R076a           | $ETE + QH = ETEP$  | K_OH_ETE                        | Table 4 |
| R077            | $OLT + OH = OLTP$  | $5.72E-12.*exp(500./T)$         | 1       |
| R077a           | $OLT + QH = OLTP$  | $5.72E-12.*exp(500./T)$         | 1       |
| R078            | $OLI + OH = OLIP$  | $1.33E-11.*exp(500./T)$         | 1       |
| R078a           | $OLI + QH = OLIP$  | $1.33E-11.*exp(500./T)$         | 1       |
| R079            | $DIEN + OH = OLIP$   | $1.48E-11.*exp(448./T)$         | 1       |
| R079a           | $DIEN + QH = OLIP$   | $1.48E-11.*exp(448./T)$         | 1       |
| R080            | $OH + ACE = 0.35ORA1 + 0.35CO + 0.35HO_2$<br>+0.65GLY+0.65OH       | K_OH_ACE                        | Table 4 |
| R080a           | $QH + ACE = 0.35ORA1 + 0.35CO + 0.35HO_2$<br>+0.65GLY+0.65OH       | K_OH_ACE                        | Table 4 |

|                  |  |                                  |   |
|------------------|--|----------------------------------|---|
| R081             | BEN+OH=0.648 HO2+0.352<br>BENP+0.118 EPX+0.53 PHEN | 2.33E-12.*exp(-193./T)           | 1 |
| R081a            | BEN+QH=0.648 HO2+0.352<br>BENP+0.118 EPX+0.53 PHEN | 2.33E-12.*exp(-193./T)           | 1 |
| R082             | TOL+OH=0.177 HO2+0.763 TR2+0.06<br>TLP1+0.177 CSL  | 1.81E-12.*exp(354./T)            | 1 |
| R082a            | TOL+QH=0.177 HO2+0.763 TR2+0.06<br>TLP1+0.177 CSL  | 1.81E-12.*exp(354./T)            | 1 |
| R083             | XYM+OH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 2.31E-11                         | 1 |
| R083a            | XYM+QH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 2.31E-11                         | 1 |
| R084             | XYP+OH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 1.43E-11                         | 1 |
| R084a            | XYP+QH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 1.43E-11                         | 1 |
| R085             | XYO+OH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 1.36E-11                         | 1 |
| R085a            | XYO+QH=0.177 HO2+0.763 XY2+0.06<br>XYL1+0.117 CSL  | 1.36E-11                         | 1 |
| R086             | ISO+OH=ISOP  | 2.54E-11.*exp(410./T)            | 1 |
| R086a            | ISO+QH=ISOP  | 2.54E-11.*exp(410./T)            | 1 |
| R087             | API+OH=APIP  | 1.21E-11.*exp(440./T)            | 1 |
| R087a            | API+QH=APIP  | 1.21E-11.*exp(440./T)            | 1 |
| R088             | LIM+OH=LIMP  | 4.20e-11.*exp(401./T)            | 1 |
| R088a            | LIM+QH=LIMP  | 4.20e-11.*exp(401./T)            | 1 |
| <b>oVOC + OH</b> |  |                                  |   |
| R089             | OH+HCHO=HO2+CO+H2O                                 | 5.50E-12.*exp(125./T)            | 1 |
| R089a            | QH+HCHO=HO2+CO+H2O                                 | 5.50E-12.*exp(125./T)            | 1 |
| R090             | OH+ACD=ACO3+H2O                                    | 4.38E-12.*exp(366./T)            | 1 |
| R090a            | QH+ACD=ACO3+H2O                                    | 4.38E-12.*exp(366./T)            | 1 |
| R091             | OH+ALD=RCO3+H2O                                    | 5.10E-12.*exp(405./T)            | 1 |
| R091a            | QH+ALD=RCO3+H2O                                    | 5.10E-12.*exp(405./T)            | 1 |
| R092             | ACT+OH=ACTP+H2O                                    | 1.39E-13+3.72E-11.*exp(-2044./T) | 1 |
| R092a            | ACT+QH=ACTP+H2O                                    | 1.39E-13+3.72E-11.*exp(-2044./T) | 1 |
| R093             | OH+MEK=MEKP+H2O                                    | 1.30E-12.*exp(-25./T)            | 1 |
| R093a            | QH+MEK=MEKP+H2O                                    | 1.30E-12.*exp(-25./T)            | 1 |
| R094             | OH+KET=KETP+H2O                                    | 2.80E-12.*exp(10./T)             | 1 |
| R094a            | QH+KET=KETP+H2O                                    | 2.80E-12.*exp(10./T)             | 1 |
| R095             | HKET+OH=HO2+MGLY+H2O                               | 3.00E-12                         | 1 |
| R095a            | HKET+QH=HO2+MGLY+H2O                               | 3.00E-12                         | 1 |
| R096             | MACR+OH=0.57 MACP+0.43 MCP                         | 8.00E-12.*exp(380./T)            | 1 |
| R096a            | MACR+QH=0.57 MACP+0.43 MCP                         | 8.00E-12.*exp(380./T)            | 1 |
| R097             | MVK+OH=MVKP  | 2.60E-12.*exp(610./T)            | 1 |

|       |  |                        |   |
|-------|--|------------------------|---|
| R097a | MVK+QH=MVKP  | 2.60E-12.*exp(610./T)  | 1 |
| R098  | UALD+OH=0.313 ACO3+0.687 UALP                                    | 5.77E-12.*exp(533./T)  | 1 |
| R098a | UALD+QH=0.313 ACO3+0.687 UALP                                    | 5.77E-12.*exp(533./T)  | 1 |
| R099  | GLY+OH=HO2+CO+CO+H2O   | 1.10E-11               | 1 |
| R099a | GLY+QH=HO2+CO+CO+H2O   | 1.10E-11               | 1 |
| R100  | MGLY+OH=ACO3+CO+H2O  | 9.26E-13.*exp(830./T)  | 1 |
| R100a | MGLY+QH=ACO3+CO+H2O  | 9.26E-13.*exp(830./T)  | 1 |
| R101  | DCB1+OH =<br>0.52HO2+0.33CO+0.40ALD+0.78KET+0<br>.10GLY+0.01MGLY | 2.80E-11.*exp(175./T)  | 1 |
| R101a | DCB1+QH =<br>0.52HO2+0.33CO+0.40ALD+0.78KET+0<br>.10GLY+0.01MGLY | 2.80E-11.*exp(175./T)  | 1 |
| R102  | DCB2+OH=<br>0.52HO2+0.33CO+0.13MEK+0.10GLY+0<br>.01MGLY+0.78OP2  | 2.80E-11.*exp(175./T)  | 1 |
| R102a | DCB2+QH=<br>0.52HO2+0.33CO+0.13MEK+0.10GLY+0<br>.01MGLY+0.78OP2  | 2.80E-11.*exp(175./T)  | 1 |
| R103  | DCB3+OH=<br>0.56HO2+0.21MACP+0.11CO+0.27GLY<br>+0.01MGLY+0.79OP2 | 1.00E-13               | 1 |
| R103a | DCB3+QH=<br>0.56HO2+0.21MACP+0.11CO+0.27GLY<br>+0.01MGLY+0.79OP2 | 1.00E-13               | 1 |
| R104  | BALD+OH=BALP+H2O   | 5.32E-12.*exp(243./T)  | 1 |
| R104a | BALD+QH=BALP+H2O   | 5.32E-12.*exp(243./T)  | 1 |
| R105  | PHEN+OH=0.73 HO2+0.20 ADDC+0.07<br>CHO+0.73 MCT                  | 6.75E-12.*exp(405./T)  | 1 |
| R105a | PHEN+QH=0.73 HO2+0.20 ADDC+0.07<br>CHO+0.73 MCT                  | 6.75E-12.*exp(405./T)  | 1 |
| R106  | CSL+OH=0.73 HO2+0.20 ADDC+0.07<br>CHO+0.73 MCT                   | 4.65E-11               | 1 |
| R106a | CSL+QH=0.73 HO2+0.20 ADDC+0.07<br>CHO+0.73 MCT                   | 4.65E-11               | 1 |
| R107  | EPX+OH=XO2+HO2+ALD+CO  | 2.80E-11.*exp(175./T)  | 1 |
| R107a | EPX+QH=XO2+HO2+ALD+CO  | 2.80E-11.*exp(175./T)  | 1 |
| R108  | MCT+OH=MCTO  | 2.05E-10               | 1 |
| R108a | MCT+QH=MCTO  | 2.05E-10               | 1 |
| R109  | OH+MOH=HO2+HCHO  | 2.85e-12.*exp(-345./T) | 1 |
| R109a | QH+MOH=HO2+HCHO  | 2.85e-12.*exp(-345./T) | 1 |
| R110  | OH+EOH=HO2+ACD   | 3.00e-12.*exp(-20./T)  | 1 |
| R110a | QH+EOH=HO2+ACD   | 3.00e-12.*exp(-20./T)  | 1 |
| R111  | OH+ROH=HO2+0.719 ALD+0.184 ACD                                   | 2.60E-12.*exp(-200./T) | 1 |
| R111a | QH+ROH=HO2+0.719 ALD+0.184 ACD                                   | 2.60E-12.*exp(-200./T) | 1 |
| R112  | ETEG+OH=ALD+HO2  | 1.47E-11               | 1 |
| R112a | ETEG+QH=ALD+HO2  | 1.47E-11               | 1 |

|       |   |                          |   |
|-------|---|--------------------------|---|
| R113  | $OP1+OH=0.35 OH+0.65 MO2+0.35 HCHO$                   | $2.90E-12.*exp(190./T)$  | 1 |
| R113a | $OP1+QH=0.35 OH+0.65 MO2+0.35 HCHO$                   | $2.90E-12.*exp(190./T)$  | 1 |
| R114  | $OP2+OH=0.49 HO+0.44 HC3P+0.07 XO2+0.08 ALD+0.41 KET$ | $3.40E-12.*exp(190./T)$  | 1 |
| R114a | $OP2+QH=0.49 HO+0.44 HC3P+0.07 XO2+0.08 ALD+0.41 KET$ | $3.40E-12.*exp(190./T)$  | 1 |
| R115  | $ISHP+OH=MACR+OH$                                     | $1.00E-10$               | 1 |
| R115a | $ISHP+QH=MACR+OH$                                     | $1.00E-10$               | 1 |
| R116  | $MAHP+OH=MACP$  | $3.00E-11$               | 1 |
| R116a | $MAHP+QH=MACP$  | $3.00E-11$               | 1 |
| R117  | $ORA1+OH=HO2+CO2+H2O$                                 | $4.50E-13$               | 1 |
| R117a | $ORA1+QH=HO2+CO2+H2O$                                 | $4.50E-13$               | 1 |
| R118  | $ORA2+OH=0.64 MO2+0.36 ORAP+0.64 CO2$                 | $2.20E-14.*exp(1012./T)$ | 1 |
| R118a | $ORA2+QH=0.64 MO2+0.36 ORAP+0.64 CO2$                 | $2.20E-14.*exp(1012./T)$ | 1 |
| R119  | $PAA+OH=0.35 HO+0.65 ACO3+0.35 XO2+0.35 HCHO$         | $2.93E-12.*exp(190./T)$  | 1 |
| R119a | $PAA+QH=0.35 HO+0.65 ACO3+0.35 XO2+0.35 HCHO$         | $2.93E-12.*exp(190./T)$  | 1 |
| R120  | $PAN+OH=XO2+NO3+HCHO+H2O$                             | $4.00E-14$               | 1 |
| R120a | $PAN+QH=XO2+NO3+HCHO+H2O$                             | $4.00E-14$               | 1 |
| R120b | $PANQ+OH=XO2+NO2Q+HCHO+H2O$                           | $4.00E-14$               | 1 |
| R120c | $PANQ+QH=XO2+NO2Q+HCHO+H2Q$                           | $4.00E-14$               | 1 |
| R120d | $PANQ2+OH=XO2+NOQ2+HCHO+H2O$                          | $4.00E-14$               | 1 |
| R120e | $PANQ2+QH=XO2+NOQ2+HCHO+H2O$                          | $4.00E-14$               | 1 |
| R121  | $PPN+OH=XO2+NO3+HCHO+H2O$                             | $4.00E-14$               | 1 |
| R121a | $PPN+QH=XO2+NO3+HCHO+H2O$                             | $4.00E-14$               | 1 |
| R121b | $PPNQ+OH=XO2+NO2Q+HCHO+H2O$                           | $4.00E-14$               | 1 |
| R121c | $PPNQ+QH=XO2+NO2Q+HCHO+H2Q$                           | $4.00E-14$               | 1 |
| R121d | $PPNQ2+OH=XO2+NOQ2+HCHO+H2O$                          | $4.00E-14$               | 1 |
| R121e | $PPNQ2+QH=XO2+NOQ2+HCHO+H2Q$                          | $4.00E-14$               | 1 |
| R122  | $MPAN+OH=HKET+NO2$                                    | $3.20E-11$               | 1 |
| R122a | $MPAN+QH=HKET+NO2$                                    | $3.20E-11$               | 1 |
| R122b | $MPANQ+OH=HKET+NO2$                                   | $3.20E-11$               | 1 |
| R122c | $MPANQ+QH=HKET+NO2$                                   | $3.20E-11$               | 1 |
| R122d | $MPANQ2+OH=HKET+NO2$                                  | $3.20E-11$               | 1 |
| R122e | $MPANQ2+QH=HKET+NO2$                                  | $3.20E-11$               | 1 |
| R123  | $ONIT+OH=HC3P+NO2+H2O$                                | $5.31E-12.*exp(-260./T)$ | 1 |
| R123a | $ONIT+QH=HC3P+NO2+H2O$                                | $5.31E-12.*exp(-260./T)$ | 1 |
| R123b | $ONITQ+OH=HC3P+(2/3)NOQ+(1/3)NO2 +H2O$                | $5.31E-12.*exp(-260./T)$ | 1 |
| R123c | $ONITQ+QH=HC3P+(2/3)NOQ+(1/3)NO2 +H2O$                | $5.31E-12.*exp(-260./T)$ | 1 |

|                            |  |                         |   |
|----------------------------|--|-------------------------|---|
| R123d                      | ONITQ2+OH=HC3P+(1/3)*NQ2+(2/3)*NOQ+H2O   | 5.31E-12.*exp(-260./T)  | 1 |
| R123e                      | ONITQ2+QH=HC3P+(1/3)*NQ2+(2/3)*NOQ+H2O   | 5.31E-12.*exp(-260./T)  | 1 |
| R123f                      | ONITQ3+OH=HC3P+NQ2+H2O   | 5.31E-12.*exp(-260./T)  | 1 |
| R123g                      | ONITQ3+QH=HC3P+NQ2+H2Q   | 5.31E-12.*exp(-260./T)  | 1 |
| R124                       | NALD+OH=NO2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R124a                      | NALD+QH=NO2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R124b                      | NALDQ+OH=(2/3)*NOQ+(1/3)*NO2+XO2+HKET  | 5.60E-12.*exp(270./T)   | 1 |
| R124c                      | NALDQ+QH=(2/3)*NOQ+(1/3)*NO2+XO2+HKET  | 5.60E-12.*exp(270./T)   | 1 |
| R124d                      | NALDQ2+OH=(2/3)*NOQ+(1/3)*NQ2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R124e                      | NALDQ2+QH=(2/3)*NOQ+(1/3)*NQ2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R124f                      | NALDQ3+OH=NQ2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R124g                      | NALDQ3+QH=NQ2+XO2+HKET   | 5.60E-12.*exp(270./T)   | 1 |
| R125                       | ISON+OH=NALD+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125a                      | ISON+QH=NALD+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125b                      | ISONQ+OH=NALDQ+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125c                      | ISONQ+QH=NALDQ+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125d                      | ISONQ2+OH=NALDQ2+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125e                      | ISONQ2+QH=NALDQ2+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125f                      | ISONQ3+OH=NALDQ3+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| R125g                      | ISONQ3+QH=NALDQ3+0.07 HKET+0.07 HCHO   | 1.30E-11                | 1 |
| <b>VOC + O<sub>3</sub></b> |  |                         |   |
| R126                       | ETE+O3=0.08QH+0.15HO2+0.43CO+HCHO+0.37ORA1+0.13H2  | 9.14E-15.*exp(-2580./T) | 1 |
| R127                       | OLT+O3=0.22QH+0.32HO2+0.08MO2+0.06ETHP+0.068H2O2+0.43CO+0.01CH4+0.02ETH+0.56HCHO+0.44ALD+0.06MEK+0.03ORA1+0.06ORA2+0.01ACD+0.01HKET+0.015HC3+0.004HC3P+0.03ACT+0.006HC5+0.02HC5P+0.02BALD+0.032BEN | 4.33E-15.*exp(-1800./T) | 1 |
| R128                       | OLI+O3=0.46QH+0.07HO2+0.32MO2+0.07ETHP   | 4.40E-15.*exp(-845./T)  | 1 |

|      |   |                         |   |
|------|---|-------------------------|---|
|      | +0.04HC3P+0.09ACO3+0.37CO+0.026H2O2+0.04CH4+0.01ETH+0.01HC3+0.09HCHO+0.457ACD+0.73ALD+0.11ACT+0.017KET+0.44HKET+0.017ORA2   |                         |   |
| R129 | DIEN+O3=0.09O3P+0.28QH+0.30HO2+0.03MO2+0.15ACO3+0.02KETP+0.13XO2+0.001H2O2+0.36CO+0.35OLT+0.90HCHO+0.39MACR+0.15ORA1+0.05H2 | 1.34E-14.*exp(-2283./T) | 1 |
| R130 | ISO+O3=0.25QH+0.25HO2+0.08MO2+0.1ACO3+0.1MACP+0.09H2O2+0.14CO+0.58HC HO+0.461MACR+0.189MVK+0.28ORA1+0.153OLT                | 7.86E-15.*exp(-1913./T) | 1 |
| R131 | API+O3=0.85QH+0.10HO2+0.20ETHP+0.42KETP+0.14CO+0.02H2O2+0.65ALD+0.53KET   | 5.00E-16.*exp(-530./T)  | 1 |
| R132 | LIM+O3=0.85QH+0.10HO2+0.16ETHP+0.42KETP+0.02H2O2+0.14CO+0.460LT+0.04HC HO+0.79MACR+0.01ORA1+0.07ORA2                        | 2.95E-15.*exp(-783./T)  | 1 |
| R133 | MACR+O3=0.19QH+0.14HO2+0.10ACO3+0.22CO+0.50MGLY+0.45ORA1  | 1.36E-15.*exp(-2112./T) | 1 |
| R134 | MVK+O3=0.16QH+0.11HO2+0.28ACO3+0.01XO2+0.56CO+0.01HCHO+0.54MGLY+0.07ORA1+0.07ORA2+0.1ALD                                    | 7.51E-16.*exp(-1520./T) | 1 |
| R135 | UALD+O3=0.1QH+0.072HO2+0.008MO2+0.002AC O3+0.1XO2+0.243CO+0.080HCHO+0.420ACD+0.028KET+0.491GLY+0.003MGLY+0.044ORA1          | 1.66E-18                | 1 |
| R136 | DCB1+O3=0.05QH+HO2+0.60RCO3+0.6XO2+1.5CO+0.05HCHO+0.05GLY+0.08MGLY+0.65OP2+0.5CO2   | 2.00E-16                | 1 |
| R137 | DCB2+O3=0.05QH+HO2+0.60RCO3+0.60XO2+1.5CO+0.05HCHO+0.05GLY+0.08MGLY+0.70DCB1+0.65OP2+0.5CO2                                 | 2.00E-16                | 1 |
| R138 | DCB3+O3 =0.05QH+HO2+1.5CO+0.48GLY+0.70DCB1+0.25ORA1+0.25ORA2+0.11PAA+1.5CO2   | 9.00E-17                | 1 |
| R139 | EPX+O3=0.05QH+1.5HO2+1.5CO+0.5CO2+GLY+0.85BALD  | 1.00E-16                | 1 |
| R140 | MCTO+O3=MCTP  | 2.86E-13                | 1 |

| Stable Organics + NO <sub>3</sub> |   |                               |   |
|-----------------------------------|---|-------------------------------|---|
| R141                              | ETE+NO3=0.80 OLNN+0.20 OLND                 | 4.88E-18.*T.^2.*exp(-2282./T) | 1 |
| R141a                             | ETE+NO2Q=0.80 OLNNQ+0.20 OLNDQ              | 4.88E-18.*T.^2.*exp(-2282./T) | 1 |
| R141b                             | ETE+NOQ2=0.80 OLNNQ2+0.20 OLNDQ2            | 4.88E-18.*T.^2.*exp(-2282./T) | 1 |
| R141c                             | ETE+NQ3=0.80 OLNNQ3+0.20 OLNDQ3             | 4.88E-18.*T.^2.*exp(-2282./T) | 1 |
| R142                              | OLT+NO3=0.43 OLNN+0.57 OLND                 | 1.79E-13.*exp(-450./T)        | 1 |
| R142a                             | OLT+NO2Q=0.43 OLNNQ+0.57 OLNDQ              | 1.79E-13.*exp(-450./T)        | 1 |
| R142b                             | OLT+NOQ2=0.43 OLNNQ2+0.57 OLNDQ2            | 1.79E-13.*exp(-450./T)        | 1 |
| R142c                             | OLT+NQ3=0.43 OLNNQ3+0.57 OLNDQ3             | 1.79E-13.*exp(-450./T)        | 1 |
| R143                              | OLI+NO3=0.11 OLNN+0.89 OLND                 | 8.64E-13.*exp(450./T)         | 1 |
| R143a                             | OLI+NO2Q=0.11 OLNNQ+0.89 OLNDQ              | 8.64E-13.*exp(450./T)         | 1 |
| R143b                             | OLI+NOQ2=0.11 OLNNQ2+0.89 OLNDQ2            | 8.64E-13.*exp(450./T)         | 1 |
| R143c                             | OLI+NQ3=0.11 OLNNQ3+0.89 OLNDQ3             | 8.64E-13.*exp(450./T)         | 1 |
| R144                              | DIEN+NO3=0.90 OLNN+0.10 OLND+0.90 MACR      | 1.0E-13                       | 1 |
| R144a                             | DIEN+NO2Q=0.90 OLNNQ+0.10 OLNDQ+0.90 MACR   | 1.0E-13                       | 1 |
| R144b                             | DIEN+NOQ2=0.90 OLNNQ2+0.10 OLNDQ2+0.90 MACR | 1.0E-13                       | 1 |
| R144c                             | DIEN+NQ3=0.90 OLNNQ3+0.10 OLNDQ3+0.90 MACR  | 1.0E-13                       | 1 |
| R145                              | ISO+NO3=ISON                                | 3.03E-12.*exp(-446./T)        | 1 |
| R145a                             | ISO+NO2Q=ISONQ                              | 3.03E-12.*exp(-446./T)        | 1 |
| R145b                             | ISO+NOQ2=ISONQ2                             | 3.03E-12.*exp(-446./T)        | 1 |
| R145c                             | ISO+NQ3=ISONQ3                              | 3.03E-12.*exp(-446./T)        | 1 |
| R146                              | API+NO3=0.10 OLNN+0.90 OLND                 | 1.19E-12.*exp(490./T)         | 1 |
| R146a                             | API+NO2Q=0.10 OLNNQ+0.90 OLNDQ              | 1.19E-12.*exp(490./T)         | 1 |
| R146b                             | API+NOQ2=0.10 OLNNQ2+0.90 OLNDQ2            | 1.19E-12.*exp(490./T)         | 1 |
| R146c                             | API+NQ3=0.10 OLNNQ2+0.90 OLNDQ3             | 1.19E-12.*exp(490./T)         | 1 |
| R147                              | LIM+NO3=0.71 OLNN+0.29 OLND                 | 1.22E-11                      | 1 |
| R147a                             | LIM+NO2Q=0.71 OLNNQ+0.29 OLNDQ              | 1.22E-11                      | 1 |
| R147b                             | LIM+NOQ2=0.71 OLNNQ2+0.29 OLNDQ2            | 1.22E-11                      | 1 |
| R147c                             | LIM+NQ3=0.71 OLNNQ3+0.29 OLNDQ3             | 1.22E-11                      | 1 |
| R148                              | HCHO+NO3=HO2+HNO3+CO                        | 2.00E-12.*exp(-2440./T)       | 1 |
| R148a                             | HCHO+NO2Q=HO2+HNO2Q+CO                      | 2.00E-12.*exp(-2440./T)       | 1 |
| R148b                             | HCHO+NOQ2=HO2+HNOQ2+CO                      | 2.00E-12.*exp(-2440./T)       | 1 |
| R148c                             | HCHO+NQ3=HO2+HNQ3+CO                        | 2.00E-12.*exp(-2440./T)       | 1 |
| R149                              | ACD+NO3=ACO3+HNO3                           | 1.40E-12.*exp(-1900./T)       | 1 |

|       |   |                           |   |
|-------|---|---------------------------|---|
| R149a | $ACD+NO2Q=ACO3+HNO2Q$   | $1.40E-12.*exp(-1900./T)$ | 1 |
| R149b | $ACD+NOQ2=ACO3+HNOQ2$   | $1.40E-12.*exp(-1900./T)$ | 1 |
| R149c | $ACD+NQ3=ACO3+HNQ3$   | $1.40E-12.*exp(-1900./T)$ | 1 |
| R150  | $ALD+NO3=RCO3+HNO3$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R150a | $ALD+NO2Q=RCO3+HNO2Q$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R150b | $ALD+NOQ2=RCO3+HNOQ2$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R150c | $ALD+NQ3=RCO3+HNQ3$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R151  | $MACR+NO3=0.32 MACP+0.68 XO2+0.32 HNO3+0.68 HCHO+0.68 MGLY+0.68 NO2$                | $3.40E-15$                | 1 |
| R151a | $MACR+NO2Q=0.32 MACP+0.68 XO2+0.32 HNO2Q+0.68 HCHO+0.68 MGLY+0.453 NOQ + 0.227 NO2$ | $3.40E-15$                | 1 |
| R151b | $MACR+NOQ2=0.32 MACP+0.68 XO2+0.32 HNOQ2+0.68 HCHO+0.68 MGLY+0.453 NOQ + 0.227 NQ2$ | $3.40E-15$                | 1 |
| R151c | $MACR+NQ3=0.32 MACP+0.68 XO2+0.32 HNQ3+0.68 HCHO+0.68 MGLY+0.68NQ2$                 | $3.40E-15$                | 1 |
| R152  | $UALD+NO3= HO2+XO2+0.668 CO+0.332 HCHO+0.332 ALD+ONIT$                              | $5.02E-13.*exp(-1076./T)$ | 1 |
| R152a | $UALD+NO2Q= HO2+XO2+0.668 CO+0.332 HCHO+0.332 ALD+ONITQ$                            | $5.02E-13.*exp(-1076./T)$ | 1 |
| R152b | $UALD+NOQ2= HO2+XO2+0.668 CO+0.332 HCHO+0.332 ALD+ONITQ2$                           | $5.02E-13.*exp(-1076./T)$ | 1 |
| R152c | $UALD+NQ3= HO2+XO2+0.668 CO+0.332 HCHO+0.332 ALD+ONITQ3$                            | $5.02E-13.*exp(-1076./T)$ | 1 |
| R153  | $GLY+NO3=HNO3+HO2+CO+CO$  | $2.90E-12.*exp(-1900./T)$ | 1 |
| R153a | $GLY+NO2Q=HNO2Q+HO2+CO+CO$  | $2.90E-12.*exp(-1900./T)$ | 1 |
| R153b | $GLY+NOQ2=HNOQ2+HO2+CO+CO$  | $2.90E-12.*exp(-1900./T)$ | 1 |
| R153c | $GLY+NQ3=HNQ3+HO2+CO+CO$  | $2.90E-12.*exp(-1900./T)$ | 1 |
| R154  | $MGLY+NO3=HNO3+ACO3+CO$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R154a | $MGLY+NO2Q=HNO2Q+ACO3+CO$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R154b | $MGLY+NOQ2=HNOQ2+ACO3+CO$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R154c | $MGLY+NQ3=HNQ3+ACO3+CO$   | $3.76E-12.*exp(-1900./T)$ | 1 |
| R155  | $PHEN+NO3=0.4 CHO+0.1 ADDC+0.5 ADCN+0.5 HNO3$                                       | $3.78E-12$                | 1 |
| R155a | $PHEN+NO2Q=0.4 CHO+0.1 ADDC+0.5 ADCNQ+0.5 HNO2Q$                                    | $3.78E-12$                | 1 |
| R155b | $PHEN+NOQ2=0.4 CHO+0.1 ADDC+0.5 ADCNQ2+0.5 HNOQ2$                                   | $3.78E-12$                | 1 |
| R155c | $PHEN+NQ3=0.4 CHO+0.1 ADDC+0.5 ADCNQ3+0.5 HNQ3$                                     | $3.78E-12$                | 1 |
| R156  | $CSL+NO3=0.4 CHO+0.1 ADDC+0.5 ADCN+0.5 HNO3$  | $1.06E-12$                | 1 |
| R156a | $CSL+NO2Q=0.4 CHO+0.1 ADDC+0.5 ADCNQ+0.5 HNO2Q$                                     | $1.06E-12$                | 1 |

|  |  |                         |   |
|--|--|-------------------------|---|
| R156b                                      | CSL+NOQ2=0.4 CHO+0.1 ADDC+0.5<br>ADCNQ2+0.5 HNOQ2                                    | 1.06E-12                | 1 |
| R156c                                      | CSL+NQ3=0.4 CHO+0.1 ADDC+0.5<br>ADCNQ3+0.5 HNQ3                                      | 1.06E-12                | 1 |
| R157                                       | EPX+NO3=0.50 HO+1.50 HO2+1.50<br>CO+0.50 CO2+GLY+0.50 NO2+0.50<br>HNO3               | 2.87E-13.*exp(-1000./T) | 1 |
| R157a                                      | EPX+NO2Q=0.50 HO+1.50 HO2+1.50<br>CO+0.50 CO2+GLY+0.33 NOQ +<br>0.166NO2 +0.50 HNO2Q | 2.87E-13.*exp(-1000./T) | 1 |
| R157b                                      | EPX+NOQ2=0.50 HO+1.50 HO2+1.50<br>CO+0.50 CO2+GLY+0.33 NOQ +<br>0.166NQ2 +0.50 HNOQ2 | 2.87E-13.*exp(-1000./T) | 1 |
| R157c                                      | EPX+NQ3=0.50 HO+1.50 HO2+1.50<br>CO+0.50 CO2+GLY+0.5 NQ2 + 0.50<br>HNQ3              | 2.87E-13.*exp(-1000./T) | 1 |
| R158                                       | MCT+NO3=MCTO+HNO3  | 2.01E-10                | 1 |
| R158a                                      | MCT+NO2Q=MCTO+HNO2Q  | 2.01E-10                | 1 |
| R158b                                      | MCT+NOQ2=MCTO+HNOQ2  | 2.01E-10                | 1 |
| R158c                                      | MCT+NQ3=MCTO+HNQ3  | 2.01E-10                | 1 |
| R159                                       | MPAN+NO3=MACP+NO2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159a                                      | MPAN+NO2Q=MACP+(2/3)NOQ +<br>(1/3)NO2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159b                                      | MPAN+NOQ2=MACP+(2/3)NOQ +<br>(1/3)NQ2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159c                                      | MPAN+NQ3=MACP+ NQ2   | 2.20E-14.*exp(-500./T)  | 1 |
| R159d                                      | MPANQ+NO3=MACP+NO2   | 2.20E-14.*exp(-500./T)  | 1 |
| R159e                                      | MPANQ+NO2Q=MACP+(2/3)NOQ +<br>(1/3)NO2   | 2.20E-14.*exp(-500./T)  | 1 |
| R159f                                      | MPANQ+NOQ2=MACP+(2/3)NOQ +<br>(1/3)NQ2   | 2.20E-14.*exp(-500./T)  | 1 |
| R159g                                      | MPANQ+NQ3=MACP+ NQ2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159h                                      | MPANQ2+NO3=MACP+NO2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159i                                      | MPANQ2+NO2Q=MACP+(2/3)NOQ +<br>(1/3)NO2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159j                                      | MPANQ2+NOQ2=MACP+(2/3)NOQ +<br>(1/3)NQ2  | 2.20E-14.*exp(-500./T)  | 1 |
| R159k                                      | MPANQ2+NQ3=MACP+ NQ2   | 2.20E-14.*exp(-500./T)  | 1 |
| <b>Aromatic Intermediate Decomposition</b> |  |                         |   |
| R160                                       | TR2=<br>0.28OH+0.29HO2+0.28TOLP+0.15PER1<br>+0.28DCB2+0.01CSL+0.28EPX                | 1.00E3                  | 1 |
| R161                                       | TOLP=<br>0.49OH+0.01HO2+0.50PER1+0.49DCB<br>2+0.01CSL                                | 1.00E3                  | 1 |
| R162                                       | XY2=<br>0.158OH+0.308HO2+0.25RCO3+0.308X   | 1.00E3                  | 1 |

|   |   |                         |         |
|---|---|-------------------------|---------|
|   | YLP+0.150PER2+0.224DCB2+0.01CSL+0.84EPX   |                         |         |
| R163  | XYLP=0.39OH+0.01HO2+0.50PER2+0.49DCB2+0.01CSL   | 1.00E3                  | 1       |
| R164  | XYO2=0.158OH+0.308HO2+0.25RCO3+0.308XYLP+0.150PER2+0.224DCB2+0.01CSL+0.84EPX                        | 1.00E3                  | 1       |
| R165  | XYOP=0.390OH+0.010HO2+0.500PER2+0.490DCB2+0.010CSL  | 1.00E3                  | 1       |
| <b>RO<sub>2</sub>NO<sub>2</sub> Formation and Decomposition</b> |   |                         |         |
| R166  | ACO3+NO2=PAN  | K_ACO3_NO2              | Table 4 |
| R166a   | ACO3+NOQ=PANQ   | K_ACO3_NO2              | Table 4 |
| R166b   | ACO3+NQ2=PANQ2  | K_ACO3_NO2              | Table 4 |
| R167  | PAN=ACO3+NO2  | K_PAN                   | Table 5 |
| R167a   | PANQ=ACO3+NOQ   | K_PAN                   | Table 5 |
| R167b   | PANQ2=ACO3+NQ2  | K_PAN                   | Table 5 |
| R168  | RCO3+NO2=PPN  | K_ACO3_NO2              | Table 4 |
| R168a   | RCO3+NOQ=PPNQ   | K_ACO3_NO2              | Table 4 |
| R168b   | RCO3+NQ2=PPNQ2  | K_ACO3_NO2              | Table 4 |
| R169  | PPN=RCO3+NO2  | K_PAN                   | Table 5 |
| R169a   | PPNQ=RCO3+NOQ   | K_PAN                   | Table 5 |
| R169b   | PPNQ2=RCO3+NQ2  | K_PAN                   | Table 5 |
| R170  | MACP+NO2=MPAN   | K_ACO3_NO2              | Table 4 |
| R170a   | MACP+NOQ=MPANQ  | K_ACO3_NO2              | Table 4 |
| R170b   | MACP+NQ2=MPANQ2   | K_ACO3_NO2              | Table 4 |
| R171  | MPAN=MACP+NO2   | 1.60E16.*exp(-13486./T) | 1       |
| R171a   | MPANQ=MACP+NOQ  | 1.60E16.*exp(-13486./T) | 1       |
| R171b   | MPANQ2=MACP+NQ2   | 1.60E16.*exp(-13486./T) | 1       |
| <b>Organic Peroxy Radicals + NO</b>                             |   |                         |         |
| R172  | MO2+NO=HCHO+HO2+NO2   | 2.80E-12.*exp(300./T)   | 1       |
| R172a   | MO2+NQ=HCHO+HO2+NOQ   | 2.80E-12.*exp(300./T)   | 1       |
| R173  | ETHP+NO=HO2+ACD+NO2   | 2.60E-12.*exp(365./T)   | 1       |
| R173a   | ETHP+NQ=HO2+ACD+NOQ   | 2.60E-12.*exp(365./T)   | 1       |
| R174  | HC3P+NO=0.66HO2+0.131MO2+0.048ETHP+0.089XO2+0.935NO2+0.504ACD+0.132ALD+0.165ACT+0.042MEK+0.065ONIT  | 4.00E-12                | 1       |
| R174a   | HC3P+NQ=0.66HO2+0.131MO2+0.048ETHP+0.089XO2+0.935NOQ+0.504ACD+0.132ALD+0.165ACT+0.042MEK+0.065ONITQ | 4.00E-12                | 1       |
| R175  | HC5P+NO=0.200HO2+0.051MO2+0.231ETHP+0.235XO2+0.864NO2+0.018HC HO+0.045ACD+0.203ALD+0.217ACT+0.      | 4.00E-12                | 1       |

|       |   |                       |   |
|-------|---|-----------------------|---|
|       | 033MEK+0.039KET+0.272HKET+0.136O<br>NIT   |                       |   |
| R175a | HC5P+NQ=0.200HO2+0.051MO2+0.23<br>1ETHP+0.235XO2+0.864NOQ+0.018HC<br>HO+0.045ACD+0.203ALD+0.217ACT+0.<br>033MEK+0.039KET+0.272HKET+0.136O<br>NITQ | 4.00E-12              | 1 |
| R176  | HC8P+NO=0.606 HO2+0.133<br>ETHP+0.416 XO2+0.739 NO2+0.150<br>ALD+0.642 KET+0.261 ONIT   | 4.00E-12              | 1 |
| R176a | HC8P+NQ=0.606 HO2+0.133<br>ETHP+0.416 XO2+0.739 NOQ+0.150<br>ALD+0.642 KET+0.261 ONITQ  | 4.00E-12              | 1 |
| R177  | ETEP+NO=HO2+NO2+1.6 HCHO+0.2<br>ALD   | 9.00E-12              | 1 |
| R177a | ETEP+NQ=HO2+NOQ+1.6 HCHO+0.2<br>ALD   | 9.00E-12              | 1 |
| R178  | OLTP+NO=0.78HO2+0.97NO2+0.78HCHO+0.012A<br>CD+0.44ALD+0.06ACT+0.13MEK+0.03O<br>NIT  | 4.00E-12              | 1 |
| R178a | OLTP+NQ=0.78HO2+0.97NOQ+0.78HCHO+0.012A<br>CD+0.44ALD+0.06ACT+0.13MEK+0.03O<br>NITQ   | 4.00E-12              | 1 |
| R179  | OLIP+NO =0.83HO2+0.95NO2+0.81ACD+0.68ALD<br>+0.20ACT+0.09KET+0.02HKET+0.05ONI<br>T  | 4.00E-12              | 1 |
| R179a | OLIP+NQ =0.83HO2+0.95NOQ+0.81ACD+0.68ALD<br>+0.20ACT+0.09KET+0.02HKET+0.05ONI<br>TQ   | 4.00E-12              | 1 |
| R180  | BENP+NO=0.918 HO2+0.918<br>NO2+0.459 DCB2+0.459 DCB3+0.918<br>GLY+0.082 ONIT  | 2.54E-12.*exp(360./T) | 1 |
| R180a | BENP+NQ=0.918 HO2+0.918<br>NOQ+0.459 DCB2+0.459 DCB3+0.918<br>GLY+0.082 ONITQ   | 2.54E-12.*exp(360./T) | 1 |
| R181  | TLP1+NO=NO2+BALD  | 4.00E-12              | 1 |
| R181a | TLP1+NQ=NOQ+BALD  | 4.00E-12              | 1 |
| R182  | TOLP+NO=0.95 HO2+0.95 NO2+0.95<br>DCB2+0.050 ONIT   | 2.70E-12.*exp(360./T) | 1 |
| R182a | TOLP+NQ=0.95 HO2+0.95 NOQ+0.95<br>DCB2+0.050 ONITQ  | 2.70E-12.*exp(360./T) | 1 |
| R183  | PER1+NO=0.5 HO2+0.95 NO2+0.5<br>BALD+0.5 MGLY+0.5 DCB1+0.05 ONIT  | 2.70E-12.*exp(360./T) | 1 |

|       |  |                       |   |
|-------|--|-----------------------|---|
| R183a | PER1+NQ=0.5 HO2+0.95 NOQ+0.5<br>BALD+0.5 MGLY+0.5 DCB1+0.05 ONITQ                              | 2.70E-12.*exp(360./T) | 1 |
| R184  | XYL1+NO=NO2+BALD   | 4.00E-12              | 1 |
| R184a | XYL1+NQ=NOQ+BALD   | 4.00E-12              | 1 |
| R185  | XYLP+NO=0.95 HO2+0.95 NO2+0.95<br>DCB3+0.050 ONIT  | 2.70E-12.*exp(360./T) | 1 |
| R185a | XYLP+NQ=0.95 HO2+0.95 NOQ+0.95<br>DCB3+0.050 ONITQ   | 2.70E-12.*exp(360./T) | 1 |
| R186  | PER2+NO=0.95 HO2+0.95 NO2+0.95<br>MGLY+0.95 DCB1+1.05 DCB3+0.05<br>ONIT                        | 2.70E-12.*exp(360./T) | 1 |
| R186a | PER2+NQ=0.95 HO2+0.95 NOQ+0.95<br>MGLY+0.95 DCB1+1.05 DCB3+0.05<br>ONITQ                       | 2.70E-12.*exp(360./T) | 1 |
| R187  | XYOP+NO=<br>0.95HO2+0.95NO2+0.350GLY+0.600M<br>GLY+0.700DCB1+0.073DCB2+0.177DC<br>B3+0.05ONIT  | 2.70E-12.*exp(360./T) | 1 |
| R187a | XYOP+NQ=<br>0.95HO2+0.95NOQ+0.350GLY+0.600M<br>GLY+0.700DCB1+0.073DCB2+0.177DC<br>B3+0.05ONITQ | 2.70E-12.*exp(360./T) | 1 |
| R188  | ISOP+NO=0.88HO2+0.88NO2+0.72HC<br>HO+0.28MACR+0.44MVK+0.12ISON+0.<br>021GLY+0.029HKET+0.27ALD  | 2.43E-12.*exp(360./T) | 1 |
| R188a | ISOP+NQ=0.88HO2+0.88NOQ+0.72HC<br>HO+0.28MACR+0.44MVK+0.12ISONQ+<br>0.021GLY+0.029HKET+0.27ALD | 2.43E-12.*exp(360./T) | 1 |
| R189  | APIP+NO=<br>0.82HO2+0.82NO2+0.23HCHO+0.43AL<br>D+0.11ACT+0.44KET+0.07ORA1+0.18O<br>NIT         | 4.00E-12              | 1 |
| R189a | APIP+NQ=<br>0.82HO2+0.82NOQ+0.23HCHO+0.43AL<br>D+0.11ACT+0.44KET+0.07ORA1+0.18O<br>NITQ        | 4.00E-12              | 1 |
| R190  | LIMP+NO=<br>HO2+NO2+0.05OLI+0.43HCHO+0.68U<br>ALD+0.07ORA1                                     | 4.00E-12              | 1 |
| R190a | LIMP+NQ=<br>HO2+NOQ+0.05OLI+0.43HCHO+0.68U<br>ALD+0.07ORA1                                     | 4.00E-12              | 1 |
| R191  | ACO3+NO=MO2+NO2  | 8.10E-12.*exp(270./T) | 1 |
| R191a | ACO3+NQ=MO2+NOQ  | 8.10E-12.*exp(270./T) | 1 |
| R192  | RCO3+NO=ETHP+NO2   | 8.10E-12.*exp(270./T) | 1 |
| R192a | RCO3+NQ=ETHP+NOQ   | 8.10E-12.*exp(270./T) | 1 |
| R193  | ACTP+NO=ACO3+NO2+HCHO  | 2.90E-12.*exp(300./T) | 1 |

|       |  |                       |   |
|-------|--|-----------------------|---|
| R193a | ACTP+NQ=ACO3+NOQ+HCHO  | 2.90E-12.*exp(300./T) | 1 |
| R194  | MEKP+NO=0.67 HO2+NO2+0.33<br>HCHO+0.67 DCB1                                | 4.00E-12              | 1 |
| R194a | MEKP+NQ=0.67 HO2+NOQ+0.33<br>HCHO+0.67 DCB1                                | 4.00E-12              | 1 |
| R195  | KETP+NO=<br>0.77HO2+0.23ACO3+0.16XO2+NO2+0.<br>54MGLY+0.46ALD              | 4.00E-12              | 1 |
| R195a | KETP+NQ=<br>0.77HO2+0.23ACO3+0.16XO2+NOQ+0.<br>54MGLY+0.46ALD              | 4.00E-12              | 1 |
| R196  | MACP+NO=0.75 HO2+0.25<br>ACO3+NO2+0.25 CO+0.75 HCHO+0.50<br>MGLY+0.25 HKET | 2.54E-12.*exp(360./T) | 1 |
| R196a | MACP+NQ=0.75 HO2+0.25<br>ACO3+NOQ+0.25 CO+0.75 HCHO+0.50<br>MGLY+0.25 HKET | 2.54E-12.*exp(360./T) | 1 |
| R197  | MCP+NO=NO2+0.50 HO2+0.50<br>HCHO+HKET                                      | 2.54E-12.*exp(360./T) | 1 |
| R197a | MCP+NQ=NOQ+0.50 HO2+0.50<br>HCHO+HKET                                      | 2.54E-12.*exp(360./T) | 1 |
| R198  | MVKP+NO=0.3 HO2+0.7 ACO3+0.7<br>XO2+NO2+0.3 HCHO+0.7 ALD+0.3<br>MGLY       | 2.54E-12.*exp(360./T) | 1 |
| R198a | MVKP+NQ=0.3 HO2+0.7 ACO3+0.7<br>XO2+NOQ+0.3 HCHO+0.7 ALD+0.3<br>MGLY       | 2.54E-12.*exp(360./T) | 1 |
| R199  | UALP+NO=<br>HO2+0.61CO+NO2+0.03HCHO+0.27AL<br>D+0.7KET+0.18GLY+0.21MGLY    | 2.54E-12.*exp(360./T) | 1 |
| R199a | UALP+NQ=<br>HO2+0.61CO+NOQ+0.03HCHO+0.27A<br>LD+0.7KET+0.18GLY+0.21MGLY    | 2.54E-12.*exp(360./T) | 1 |
| R200  | BALP+NO=BAL1+NO2   | 4.00E-12              | 1 |
| R200a | BALP+NQ=BAL1+NOQ   | 4.00E-12              | 1 |
| R201  | BAL1+NO=BAL2+NO2   | 4.00E-12              | 1 |
| R201a | BAL1+NQ=BAL2+NOQ   | 4.00E-12              | 1 |
| R202  | ADDC+NO=HO2+NO2+0.32 HKET+0.68<br>GLY+0.68 OP2                             | 2.70E-12.*exp(360./T) | 1 |
| R202a | ADDC+NQ=HO2+NOQ+0.32 HKET+0.68<br>GLY+0.68 OP2                             | 2.70E-12.*exp(360./T) | 1 |
| R203  | MCTP+NO=MCTO+NO2   | 2.70E-12.*exp(360./T) | 1 |
| R203a | MCTP+NQ=MCTO+NOQ   | 2.70E-12.*exp(360./T) | 1 |
| R204  | ORAP+NO=HO2+NO2+GLY  | 4.00E-12              | 1 |
| R204a | ORAP+NQ=HO2+NOQ+GLY  | 4.00E-12              | 1 |
| R205  | OLNN+NO=ONIT+NO2+HO2   | 4.00E-12              | 1 |
| R205a | OLNN+NQ=ONIT+NOQ+HO2   | 4.00E-12              | 1 |

|       |   |                       |   |
|-------|---|-----------------------|---|
| R205b | OLNNQ+NO=ONITQ+NO2+HO2  | 4.00E-12              | 1 |
| R205c | OLNNQ+NQ=ONITQ+NOQ+HO2  | 4.00E-12              | 1 |
| R205d | OLNNQ2+NO=ONITQ2+NO2+HO2                                      | 4.00E-12              | 1 |
| R205e | OLNNQ2+NQ=ONITQ2+NOQ+HO2                                      | 4.00E-12              | 1 |
| R205f | OLNNQ3+NO=ONITQ3+NO2+HO2                                      | 4.00E-12              | 1 |
| R205g | OLNNQ3+NQ=ONITQ3+NOQ+HO2                                      | 4.00E-12              | 1 |
| R206  | OLND+NO=2NO2+0.287HCHO+1.24ALD+0.464KET                       | 4.00E-12              | 1 |
| R206a | OLND+NQ=NO2+NOQ+0.287HCHO+1.24ALD+0.464KET                    | 4.00E-12              | 1 |
| R206b | OLNDQ+NO=(2/3)NO2+(1/3)NOQ+NO2+0.287HCHO+1.24ALD+0.464KET     | 4.00E-12              | 1 |
| R206c | OLNDQ+NQ=(2/3)NO2+(1/3)NOQ+NO2+NOQ+0.287HCHO+1.24ALD+0.464KET | 4.00E-12              | 1 |
| R206d | OLNDQ2+NO=(2/3)NOQ+(1/3)NQ2+NO2+0.287HCHO+1.24ALD+0.464KET    | 4.00E-12              | 1 |
| R206e | OLNDQ2+NQ=(2/3)NOQ+(1/3)NQ2+NOQ+0.287HCHO+1.24ALD+0.464KET    | 4.00E-12              | 1 |
| R206f | OLNDQ3+NO=NQ2+NO2+0.287HCHO+1.24ALD+0.464KET                  | 4.00E-12              | 1 |
| R206g | OLNDQ3+NQ=NQ2+NOQ+0.287HCHO+1.24ALD+0.464KET                  | 4.00E-12              | 1 |
| R207  | ADCN+NO=GLY+NO2+NO2+OP2                                       | 2.70E-12.*exp(360./T) | 1 |
| R207a | ADCN+NQ=GLY+NO2+NOQ+OP2                                       | 2.70E-12.*exp(360./T) | 1 |
| R207b | ADCNQ+NO=GLY+(2/3)NOQ+(1/3)NO2+NO2+OP2                        | 2.70E-12.*exp(360./T) | 1 |
| R207c | ADCNQ+NQ=GLY+(2/3)NOQ+(1/3)NO2+NOQ+OP2                        | 2.70E-12.*exp(360./T) | 1 |
| R207d | ADCNQ2+NO=GLY+(2/3)NOQ+(1/3)NQ2+NO2+OP2                       | 2.70E-12.*exp(360./T) | 1 |
| R207e | ADCNQ2+NQ=GLY+(2/3)NOQ+(1/3)NQ2+NOQ+OP2                       | 2.70E-12.*exp(360./T) | 1 |
| R207f | ADCNQ3+NO=GLY+NQ2+NO2+OP2                                     | 2.70E-12.*exp(360./T) | 1 |
| R207g | ADCNQ3+NQ=GLY+NQ2+NOQ+OP2                                     | 2.70E-12.*exp(360./T) | 1 |
| R208  | XO2+NO=NO2  | 4.00E-12              | 1 |
| R208a | XO2+NQ=NOQ  | 4.00E-12              | 1 |

#### Organic Termination with Nitrogen Dioxide

|       |                 |          |   |
|-------|-----------------|----------|---|
| R209  | BAL2+NO2=ONIT   | 2.00E-11 | 1 |
| R209a | BAL2+NOQ=ONITQ  | 2.00E-11 | 1 |
| R209b | BAL2+NQ2=ONITQ2 | 2.00E-11 | 1 |
| R210  | CHO+NO2=ONIT    | 2.00E-11 | 1 |
| R210a | CHO+NOQ=ONITQ   | 2.00E-11 | 1 |
| R210b | CHO+NQ2=ONITQ2  | 2.00E-11 | 1 |
| R211  | MCTO+NO2=ONIT   | 2.08E-12 | 1 |
| R211a | MCTO+NOQ=ONITQ  | 2.08E-12 | 1 |
| R211b | MCTO+NQ2=ONITQ2 | 2.08E-12 | 1 |

| Organic Peroxy Radicals + HO <sub>2</sub> |              |                        |   |
|---|--------------|------------------------|---|
| R212                                      | MO2+HO2=OP1  | 4.10E-13.*exp(750./T)  | 1 |
| R212a                                     | MO2+HOQ=OP1  | 4.10E-13.*exp(750./T)  | 1 |
| R212b                                     | MO2+H2Q=OP1  | 4.10E-13.*exp(750./T)  | 1 |
| R213                                      | ETHP+HO2=OP2 | 7.50E-13.*exp(700./T)  | 1 |
| R213a                                     | ETHP+HOQ=OP2 | 7.50E-13.*exp(700./T)  | 1 |
| R213b                                     | ETHP+HQ2=OP2 | 7.50E-13.*exp(700./T)  | 1 |
| R214                                      | HC3P+HO2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R214a                                     | HC3P+HOQ=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R214b                                     | HC3P+HQ2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R215                                      | HC5P+HO2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R215a                                     | HC5P+HOQ=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R215b                                     | HC5P+HQ2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R216                                      | HC8P+HO2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R216a                                     | HC8P+HOQ=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R216b                                     | HC8P+HQ2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R217                                      | ETEP+HO2=OP2 | 1.90E-13.*exp(1300./T) | 1 |
| R217a                                     | ETEP+HOQ=OP2 | 1.90E-13.*exp(1300./T) | 1 |
| R217b                                     | ETEP+HQ2=OP2 | 1.90E-13.*exp(1300./T) | 1 |
| R218                                      | OLTP+HO2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R218a                                     | OLTP+HOQ=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R218b                                     | OLTP+HQ2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R219                                      | OLIP+HO2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R219a                                     | OLIP+HOQ=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R219b                                     | OLIP+HQ2=OP2 | 1.66E-13.*exp(1300./T) | 1 |
| R220                                      | BENP+HO2=OP2 | 2.91E-13.*exp(1300./T) | 1 |
| R220a                                     | BENP+HOQ=OP2 | 2.91E-13.*exp(1300./T) | 1 |
| R220b                                     | BENP+HQ2=OP2 | 2.91E-13.*exp(1300./T) | 1 |
| R221                                      | TLP1+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R221a                                     | TLP1+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R221b                                     | TLP1+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R222                                      | TOLP+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R222a                                     | TOLP+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R222b                                     | TOLP+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R223                                      | PER1+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R223a                                     | PER1+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R223b                                     | PER1+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R224                                      | XYL1+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R224a                                     | XYL1+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R224b                                     | XYL1+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R225                                      | XYLP+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R225a                                     | XYLP+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R225b                                     | XYLP+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R226                                      | PER2+HO2=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R226a                                     | PER2+HOQ=OP2 | 3.75E-13.*exp(980./T)  | 1 |
| R226b                                     | PER2+HQ2=OP2 | 3.75E-13.*exp(980./T)  | 1 |

|       |   |                        |   |
|-------|---|------------------------|---|
| R227  | XYOP+HO2=OP2  | 3.75E-13.*exp(980./T)  | 1 |
| R227a | XYOP+HOQ=OP2  | 3.75E-13.*exp(980./T)  | 1 |
| R227b | XYOP+HQ2=OP2  | 3.75E-13.*exp(980./T)  | 1 |
| R228  | ISOP+HO2=ISHP   | 2.05E-13.*exp(1300./T) | 1 |
| R228a | ISOP+HOQ=ISHP   | 2.05E-13.*exp(1300./T) | 1 |
| R228b | ISOP+HQ2=ISHP   | 2.05E-13.*exp(1300./T) | 1 |
| R229  | APIP+HO2=OP2  | 1.50E-11               | 1 |
| R229a | APIP+HOQ=OP2  | 1.50E-11               | 1 |
| R229b | APIP+HQ2=OP2  | 1.50E-11               | 1 |
| R230  | LIMP+HO2=OP2  | 1.50E-11               | 1 |
| R230a | LIMP+HOQ=OP2  | 1.50E-11               | 1 |
| R230b | LIMP+HQ2=OP2  | 1.50E-11               | 1 |
| R231  | ACO3+HO2=0.44 HO+0.44 MO2+0.44<br>CO2+0.15 ORA2+0.41 PAA  | 4.30E-13.*exp(1040./T) | 1 |
| R231a | ACO3+HOQ=0.44 HO+0.44 MO2+0.44<br>CO2+0.15 ORA2+0.41 PAA  | 4.30E-13.*exp(1040./T) | 1 |
| R231b | ACO3+HQ2=0.44 HO+0.44 MO2+0.44<br>CO2+0.15 ORA2+0.41 PAA  | 4.30E-13.*exp(1040./T) | 1 |
| R232  | RCO3+HO2=0.44 HO+0.44 ETPH+0.44<br>CO2+0.15 ORA2+0.41 PAA | 4.30E-13.*exp(1040./T) | 1 |
| R232a | RCO3+HOQ=0.44 HO+0.44 ETPH+0.44<br>CO2+0.15 ORA2+0.41 PAA | 4.30E-13.*exp(1040./T) | 1 |
| R232b | RCO3+HQ2=0.44 HO+0.44 ETPH+0.44<br>CO2+0.15 ORA2+0.41 PAA | 4.30E-13.*exp(1040./T) | 1 |
| R233  | ACTP+HO2= 0.15 HO+0.15 ACO3+0.15<br>HCHO+0.850 OP2        | 1.15E-13.*exp(1300./T) | 1 |
| R233a | ACTP+HOQ= 0.15 HO+0.15 ACO3+0.15<br>HCHO+0.850 OP2        | 1.15E-13.*exp(1300./T) | 1 |
| R233b | ACTP+HQ2= 0.15 HO+0.15 ACO3+0.15<br>HCHO+0.850 OP2        | 1.15E-13.*exp(1300./T) | 1 |
| R234  | MEKP+HO2=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R234a | MEKP+HOQ=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R234b | MEKP+HQ2=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R235  | KETP+HO2=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R235a | KETP+HOQ=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R235b | KETP+HQ2=OP2  | 1.15E-13.*exp(1300./T) | 1 |
| R236  | MACP+HO2=MAHP   | 1.82E-13.*exp(1300./T) | 1 |
| R236a | MACP+HOQ=MAHP   | 1.82E-13.*exp(1300./T) | 1 |
| R236b | MACP+HQ2=MAHP   | 1.82E-13.*exp(1300./T) | 1 |
| R237  | MCP+HO2=MAHP  | 1.82E-13.*exp(1300./T) | 1 |
| R237a | MCP+HOQ=MAHP  | 1.82E-13.*exp(1300./T) | 1 |
| R237b | MCP+HQ2=MAHP  | 1.82E-13.*exp(1300./T) | 1 |
| R238  | MVKP+HO2=OP2  | 7.70E-14.*exp(1298./T) | 1 |
| R238a | MVKP+HOQ=OP2  | 7.70E-14.*exp(1298./T) | 1 |
| R238b | MVKP+HQ2=OP2  | 7.70E-14.*exp(1298./T) | 1 |
| R239  | UALP+HO2=OP2  | 7.70E-14.*exp(1298./T) | 1 |

|       |                   |                        |   |
|-------|-------------------|------------------------|---|
| R239a | UALP+HOQ=OP2      | 7.70E-14.*exp(1298./T) | 1 |
| R239b | UALP+HQ2=OP2      | 7.70E-14.*exp(1298./T) | 1 |
| R240  | ADDC+HO2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R240a | ADDC+HOQ=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R240b | ADDC+HQ2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R241  | CHO+HO2=CSL       | 1.00E-11               | 1 |
| R241a | CHO+HOQ=CSL       | 1.00E-11               | 1 |
| R241b | CHO+HQ2=CSL       | 1.00E-11               | 1 |
| R242  | MCTP+HO2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R242a | MCTP+HOQ=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R242b | MCTP+HQ2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R243  | ORAP+HO2=ONIT     | 1.15E-13.*exp(1300./T) | 1 |
| R243a | ORAP+HOQ=ONIT     | 1.15E-13.*exp(1300./T) | 1 |
| R243b | ORAP+HQ2=ONIT     | 1.15E-13.*exp(1300./T) | 1 |
| R244  | OLNN+HO2=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R244a | OLNN+HOQ=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R244b | OLNN+HQ2=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R244c | OLNNQ+HO2=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R244d | OLNNQ+HOQ=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R244e | OLNNQ+HQ2=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R244f | OLNNQ2+HO2=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R244g | OLNNQ2+HOQ=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R244h | OLNNQ2+HQ2=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R244i | OLNNQ3+HO2=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R244j | OLNNQ3+HOQ=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R244k | OLNNQ3+HQ2=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R245  | OLND+HO2=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R245a | OLND+HOQ=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R245b | OLND+HQ2=ONIT     | 1.66E-13.*exp(1300./T) | 1 |
| R245c | OLNDQ+HO2=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R245d | OLNDQ+HOQ=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R245e | OLNDQ+HQ2=ONITQ   | 1.66E-13.*exp(1300./T) | 1 |
| R245f | OLNDQ2+HO2=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R245g | OLNDQ2+HOQ=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R245h | OLNDQ2+HQ2=ONITQ2 | 1.66E-13.*exp(1300./T) | 1 |
| R245i | OLNDQ3+HO2=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R245j | OLNDQ3+HOQ=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R245k | OLNDQ3+HQ2=ONITQ3 | 1.66E-13.*exp(1300./T) | 1 |
| R246  | ADCN+HO2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R246a | ADCN+HOQ=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R246b | ADCN+HQ2=OP2      | 3.75E-13.*exp(980./T)  | 1 |
| R246c | ADCNQ+HO2=OP2     | 3.75E-13.*exp(980./T)  | 1 |
| R246d | ADCNQ+HOQ=OP2     | 3.75E-13.*exp(980./T)  | 1 |
| R246e | ADCNQ+HQ2=OP2     | 3.75E-13.*exp(980./T)  | 1 |
| R246f | ADCNQ2+HO2=OP2    | 3.75E-13.*exp(980./T)  | 1 |
| R246g | ADCNQ2+HOQ=OP2    | 3.75E-13.*exp(980./T)  | 1 |

|   |  |                        |   |
|---|--|------------------------|---|
| R246h   | ADCNQ2+HQ2=OP2   | 3.75E-13.*exp(980./T)  | 1 |
| R246i   | ADCNQ3+HO2=OP2   | 3.75E-13.*exp(980./T)  | 1 |
| R246j   | ADCNQ3+HOQ=OP2   | 3.75E-13.*exp(980./T)  | 1 |
| R246k   | ADCNQ3+HQ2=OP2   | 3.75E-13.*exp(980./T)  | 1 |
| R247  | XO2+HO2=OP2  | 1.66E-13.*exp(1300./T) | 1 |
| R247a   | XO2+HOQ=OP2  | 1.66E-13.*exp(1300./T) | 1 |
| R247b   | XO2+HQ2=OP2  | 1.66E-13.*exp(1300./T) | 1 |
| <b>Organic Peroxy Radicals + Methyl Peroxy Radicals</b> |  |                        |   |
| R248  | MO2+MO2=0.74 HO2+1.37 HCHO+0.63 MOH  | 9.50E-14.*exp(390./T)  | 1 |
| R249  | ETHP+MO2=HO2+0.75 HCHO+0.75 ACD+0.25 MOH+0.25 EOH  | 1.18E-13.*exp(158./T)  | 1 |
| R250  | HC3P+MO2=0.894HO2+0.080MO2+0.026ETHP+0.026XO2+0.827HCHO+0.198ALD+0.497KET+0.050GLY+0.25MOH+0.25ROH | 9.46E-14.*exp(431./T)  | 1 |
| R251  | HC5P+MO2=0.842HO2+0.018MO2+0.14ETHP+0.191XO2+0.777HCHO+0.251ALD+0.618KET+0.25MOH+0.25ROH           | 1.00E-13.*exp(467./T)  | 1 |
| R252  | HC8P+MO2=0.910HO2+0.090ETHP+0.281XO2+0.750HCHO+0.197ALD+0.652KET+0.250MOH+0.250ROH                 | 4.34E-14.*exp(633./T)  | 1 |
| R253  | ETEP+MO2=HO2+1.95HCHO+0.15ALD+0.25MOH+0.25ETEG   | 1.71E-13.*exp(708./T)  | 1 |
| R254  | OLTP+MO2=HO2+1.5HCHO+0.705ALD+0.045KET+0.25MOH+0.25ROH   | 1.46E-13.*exp(708./T)  | 1 |
| R255  | OLIP+MO2=HO2+0.75HCHO+1.28ALD+0.218KET+0.250MOH+0.250ROH   | 9.18E-14.*exp(708./T)  | 1 |
| R256  | BENP+MO2=1.6HO2+0.459DCB3+HCHO+0.459DCB2+0.6GLY  | 3.56E-14.*exp(708./T)  | 1 |
| R257  | TLP1+MO2=HCHO+HO2+BALD   | 3.56E-14.*exp(708./T)  | 1 |
| R258  | TOLP+MO2=2 HO2+HCHO+0.271GLY+DCB2  | 3.56E-14.*exp(708./T)  | 1 |
| R259  | PER1+MO2=HCHO+HO2+HO2+MGLY+DCB1  | 3.56E-14.*exp(708./T)  | 1 |
| R260  | XYL1+MO2=HCHO+HO2+BALD   | 3.56E-14.*exp(708./T)  | 1 |
| R261  | XYLP+MO2=HCHO+HO2+HO2+DCB2   | 3.56E-14.*exp(708./T)  | 1 |
| R262  | PER2+MO2=HCHO+HO2+HO2+MGLY+DCB1+1.05DCB3   | 3.56E-14.*exp(708./T)  | 1 |

|       |   |                                      |   |
|-------|---|--------------------------------------|---|
| R263  | $\text{XYOP} + \text{MO}_2 = 2\text{HO}_2 + \text{HCHO} + 0.368\text{GLY} + 0.632\text{MGLY} + 0.737\text{DCB1} + 0.077\text{DCB2} + 0.186\text{DCB3}$                                      | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R264  | $\text{ISOP} + \text{MO}_2 = \text{HO}_2 + 1.31\text{HCHO} + 0.159\text{MA CR} + 0.250\text{MVK} + 0.250\text{MOH} + 0.250\text{ROH} + 0.23\text{ALD} + 0.018\text{GLY} + 0.016\text{HKET}$ | $3.40\text{E-14} \cdot \exp(221./T)$ | 1 |
| R265  | $\text{APIP} + \text{MO}_2 = \text{HO}_2 + 0.75\text{ HCHO} + 0.75\text{ ALD} + 0.75\text{ KET} + 0.25\text{ MOH} + 0.25\text{ ROH}$  | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R266  | $\text{LIMP} + \text{MO}_2 = \text{HO}_2 + 0.192\text{OLI} + 1.04\text{HCHO} + 0.308\text{MAC R} + 0.25\text{MOH} + 0.25\text{ROH}$   | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R267  | $\text{ACO}_3 + \text{MO}_2 = 0.9\text{HO}_2 + 0.9\text{MO}_2 + 0.4\text{CO}_2 + \text{HCHO} + 0.1\text{ORA2}$  | $2.00\text{E-12} \cdot \exp(500./T)$ | 2 |
| R268  | $\text{RCO}_3 + \text{MO}_2 = 0.9\text{HO}_2 + 0.9\text{MO}_2 + 0.4\text{CO}_2 + \text{HCHO} + 0.1\text{ORA2}$  | $2.00\text{E-12} \cdot \exp(500./T)$ | 2 |
| R269  | $\text{ACTP} + \text{MO}_2 = 0.5\text{ HO}_2 + 0.5\text{ ACO}_3 + 1.5\text{ HCHO} + 0.25\text{ MOH} + 0.25\text{ ROH} + 0.125\text{ ORA2}$  | $7.50\text{E-13} \cdot \exp(500./T)$ | 1 |
| R270  | $\text{MEKP} + \text{MO}_2 = 0.834\text{ HO}_2 + \text{HCHO} + 0.334\text{ DCB1} + 0.25\text{ MOH} + 0.25\text{ ROH}$   | $6.91\text{E-13} \cdot \exp(508./T)$ | 1 |
| R271  | $\text{KETP} + \text{MO}_2 = \text{HO}_2 + 0.75\text{ HCHO} + 0.50\text{ DCB1} + 0.25\text{ MOH} + 0.25\text{ ROH}$   | $6.91\text{E-13} \cdot \exp(508./T)$ | 1 |
| R272  | $\text{MACP} + \text{MO}_2 = 0.5\text{HO}_2 + 0.269\text{ACO}_3 + 0.5\text{C O} + 1.66\text{HCHO} + 0.250\text{MOH} + 0.250\text{ROH} + 0.067\text{ORA2} + 0.25\text{MO2}$                  | $3.40\text{E-14} \cdot \exp(221./T)$ | 1 |
| R273  | $\text{MCP} + \text{MO}_2 = \text{NO}_2 + \text{HO}_2 + 1.5\text{ HCHO} + 0.5\text{ HKET} + 0.25\text{ MOH} + 0.25\text{ ROH}$  | $3.40\text{E-14} \cdot \exp(221./T)$ | 1 |
| R274  | $\text{MVKP} + \text{MO}_2 = \text{HO}_2 + 1.16\text{ACO}_3 + 1.16\text{XO}_2 + 1.5\text{HCHO} + 1.75\text{ALD} + 0.50\text{MGLY} + 0.25\text{MOH} + 0.25\text{ROH} + 0.292\text{ORA2}$     | $3.40\text{E-14} \cdot \exp(221./T)$ | 1 |
| R275  | $\text{UALP} + \text{MO}_2 = \text{HO}_2 + 0.305\text{CO} + 0.773\text{HCHO} + 0.203\text{ALD} + 0.525\text{KET} + 0.105\text{MGLY} + 0.135\text{GLY} + 0.25\text{ MOH} + 0.25\text{ROH}$   | $3.40\text{E-14} \cdot \exp(221./T)$ | 1 |
| R276  | $\text{BALP} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{BAL1}$   | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R277  | $\text{BAL1} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{BAL2}$   | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R278  | $\text{ADDC} + \text{MO}_2 = 2\text{ HO}_2 + \text{HCHO} + 0.32\text{ HKET} + 0.68\text{ GLY} + 0.68\text{ OP2}$  | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R279  | $\text{MCTP} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{MCTO}$   | $3.56\text{E-14} \cdot \exp(708./T)$ | 1 |
| R280  | $\text{ORAP} + \text{MO}_2 = \text{HO}_2 + \text{HCHO} + \text{GLY}$  | $7.50\text{E-13} \cdot \exp(500./T)$ | 1 |
| R281  | $\text{OLNN} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{HO}_2 + \text{ONIT}$   | $1.60\text{E-13} \cdot \exp(708./T)$ | 1 |
| R281a | $\text{OLNNQ} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{HO}_2 + \text{ONIT Q}$  | $1.60\text{E-13} \cdot \exp(708./T)$ | 1 |
| R281b | $\text{OLNNQ2} + \text{MO}_2 = \text{HCHO} + \text{HO}_2 + \text{HO}_2 + \text{ONI TQ2}$  | $1.60\text{E-13} \cdot \exp(708./T)$ | 1 |

|  |  |                        |   |
|--|--|------------------------|---|
| R281c  | OLNNQ3+MO2=HCHO+HO2+HO2+ONITQ3   | 1.60E-13.*exp(708./T)  | 1 |
| R282   | OLND+MO2=0.50HO2+0.50NO2+0.965HCHO+0.93ALD+0.348KET+0.25MOH+0.25ROH+0.5ONIT                  | 9.68E-14.*exp(708./T)  | 1 |
| R282a  | OLNDQ+MO2=0.50HO2+0.25NOQ+0.25NO2+0.965HC HO+0.93ALD+0.348KET+0.25MOH+0.25ROH+0.5ONITQ       | 9.68E-14.*exp(708./T)  | 1 |
| R282b  | OLNDQ2+MO2=0.50HO2+0.25NOQ+0.25NQ2+0.965HC HO+0.93ALD+0.348KET+0.25MOH+0.25ROH+0.5ONITQ2     | 9.68E-14.*exp(708./T)  | 1 |
| R282c  | OLNDQ3+MO2=0.50HO2+0.5NQ2+0.965HCHO+0.93ALD+0.348KET+0.25MOH+0.25ROH+0.5ONITQ3               | 9.68E-14.*exp(708./T)  | 1 |
| R283   | ADCN+MO2=HO2+0.7 NO2+HCHO+0.7 GLY+0.7 OP2+0.3 ONIT   | 3.56E-14               | 1 |
| R283a  | ADCNQ+MO2=HO2+0.4667 NOQ + 0.233 NO2 +HCHO+0.7 GLY+0.7 OP2+0.3 ONITQ                         | 3.56E-14               | 1 |
| R283b  | ADCNQ2+MO2=HO2+0.4667 NOQ + 0.233 NQ2 +HCHO+0.7 GLY+0.7 OP2+0.3 ONITQ2                       | 3.56E-14               | 1 |
| R283c  | ADCNQ3+MO2=HO2+0.7 NQ2 +HCHO+0.7 GLY+0.7 OP2+0.3 ONITQ3                                      | 3.56E-14               | 1 |
| R284   | XO2+MO2=HCHO+HO2   | 5.99E-15.*exp(1510./T) | 1 |
| <b>Organic Peroxy Radicals + Acetyl Peroxy Radical</b> |  |                        |   |
| R285   | ETHP+ACO3=0.500 HO2+0.5 MO2+ACD+0.5 ORA2   | 1.03E-12.*exp(211./T)  | 1 |
| R286   | HC3P+ACO3=0.394HO2+0.580MO2+0.026ETHP+0.026XO2+0.130HCHO+0.273ALD+0.662KET+0.067GLY+0.50ORA2 | 6.90E-13.*exp(460./T)  | 1 |
| R287   | HC5P+ACO3=0.342HO2+0.518MO2+0.140ETHP+0.191XO2+0.042HCHO+0.381ALD+0.824KET+0.50ORA2          | 5.59E-13.*exp(522./T)  | 1 |
| R288   | HC8P+ACO3=0.303HO2+0.5MO2+0.067ETHP+0.208XO2+0.217ALD+0.642KET+0.495ORA2                     | 2.47E-13.*exp(683./T)  | 1 |
| R289   | ETEP+ACO3=0.5 HO2+0.5 MO2+1.6 HCHO+0.2 ALD+0.5 ORA2  | 9.48E-13.*exp(765./T)  | 1 |

|      |  |                       |   |
|------|--|-----------------------|---|
| R290 | OLTP+ACO3=0.50 HO2+0.50<br>MO2+HCHO+0.94 ALD+0.06 KET+0.50<br>ORA2                             | 8.11E-13.*exp(765./T) | 1 |
| R291 | OLIP+ACO3=0.50 HO2+0.50 MO2+1.71<br>ALD+0.29 KET+0.50 ORA2                                     | 5.09E-13.*exp(765./T) | 1 |
| R292 | BENP+ACO3=<br>0.60HO2+MO2+0.459DCB2+0.458DCB<br>3+0.60GLY                                      | 7.40E-13.*exp(765./T) | 1 |
| R293 | TLP1+ACO3=MO2+BALD   | 7.40E-13.*exp(765./T) | 1 |
| R294 | TOLP+ACO3=DCB2+HO2+MO2   | 7.40E-13.*exp(765./T) | 1 |
| R295 | PER1+ACO3=DCB1+MO2+MGLY+HO2  | 7.40E-13.*exp(765./T) | 1 |
| R296 | XYL1+ACO3=MO2+BALD   | 7.40E-13.*exp(765./T) | 1 |
| R297 | XYLP+ACO3=DCB2+MO2+HO2   | 7.40E-13.*exp(765./T) | 1 |
| R298 | PER2+ACO3=DCB1+MO2+MGLY+HO2+<br>1.05DCB3   | 7.40E-13.*exp(765./T) | 1 |
| R299 | XYOP+ACO3= HO2+MO2+0.368<br>GLY+0.632 MGLY+0.737 DCB1+0.077<br>DCB2+0.186 DCB3                 | 7.40E-13.*exp(765./T) | 1 |
| R300 | ISOP+ACO3=0.5HO2+0.5MO2+0.75HC<br>HO+0.159MACR+0.25MVK+0.5ORA2+0.<br>031ALD+0.024GLY+0.033HKET | 8.40E-14.*exp(221./T) | 1 |
| R301 | APIP+ACO3=0.5 HO2+0.5<br>MO2+ALD+KET+ORA2  | 7.40E-13.*exp(765./T) | 1 |
| R302 | LIMP+ACO3=0.5 HO2+0.5 MO2+0.192<br>OLI+0.385 HCHO+0.308 MACR+0.5<br>ORA2                       | 7.40E-13.*exp(765./T) | 1 |
| R303 | ACO3+ACO3=MO2+MO2+CO2+CO2  | 2.50E-12.*exp(500./T) | 1 |
| R304 | RCO3+ACO3=MO2+EHTP+CO2+CO2   | 2.50E-12.*exp(500./T) | 1 |
| R305 | ACTP+ACO3=0.50 MO2+0.50<br>ACO3+HCHO+0.75 ORA2   | 7.51E-13.*exp(565./T) | 1 |
| R306 | MEKP+ACO3=0.33 HO2+0.50 MO2+0.33<br>HCHO+0.334 DCB1+0.50 ORA2                                  | 7.51E-13.*exp(565./T) | 1 |
| R307 | KETP+ACO3=0.50 HO2+0.50 MO2+0.50<br>DCB1+0.50 ORA2   | 7.51E-13.*exp(565./T) | 1 |
| R308 | MACP+ACO3=<br>0.50HO2+0.50MO2+0.167ACO3+0.167<br>CO+HCHO+0.167HKET+0.33MGLY+0.5<br>83ORA2      | 8.40E-14.*exp(221./T) | 1 |
| R309 | MCP+ACO3=NO2+0.5 HO2+HCHO +0.5<br>HKET+0.5 MO2+0.5 ORA2  | 8.40E-14.*exp(221./T) | 1 |
| R310 | MVKP+ACO3=<br>0.5HO2+0.5MO2+1.16ACO3+1.16XO2+<br>HCHO+2.3ALD+0.5MGLY+1.083ORA2                 | 8.40E-14.*exp(221./T) | 1 |
| R311 | UALP+ACO3=<br>0.5HO2+0.5MO2+0.5CO+0.030HCHO+<br>0.27ALD+0.70KET+0.18GLY+0.105MGLY<br>+0.5ORA2  | 8.40E-14.*exp(221./T) | 1 |

|       |   |                        |   |
|-------|---|------------------------|---|
| R312  | BALP+ACO3=BAL1+MO2  | 7.40E-13.*exp(765./T)  | 1 |
| R313  | BAL1+ACO3=BAL2+MO2  | 7.40E-13.*exp(765./T)  | 1 |
| R314  | ADDC+ACO3=2 HO2+MO2+0.32<br>HKET+0.68 GLY+0.68 OP2                                  | 7.40E-13.*exp(708./T)  | 1 |
| R315  | MCTP+ACO3=MO2+HO2+MCTO  | 7.40E-13.*exp(708./T)  | 1 |
| R316  | ORAP+ACO3=MO2+GLY   | 7.51E-13.*exp(565./T)  | 1 |
| R317  | OLNN+ACO3=ONIT+MO2+HO2  | 8.85E-13.*exp(765./T)  | 1 |
| R317a | OLNNQ+ACO3=ONITQ+MO2+HO2  | 8.85E-13.*exp(765./T)  | 1 |
| R317b | OLNNQ2+ACO3=ONITQ2+MO2+HO2  | 8.85E-13.*exp(765./T)  | 1 |
| R317c | OLNNQ3+ACO3=ONITQ3+MO2+HO2  | 8.85E-13.*exp(765./T)  | 1 |
| R318  | OLND+ACO3=<br>0.50MO2+NO2+0.287HCHO+1.24ALD+<br>0.464KET+0.50ORA2                   | 5.37E-13.*exp(765./T)  | 1 |
| R318a | OLNDQ+ACO3=<br>0.50MO2+(1/3)*NO2+(2/3)*NOQ+0.287<br>HCHO+1.24ALD+0.464KET+0.50ORA2  | 5.37E-13.*exp(765./T)  | 1 |
| R318b | OLNDQ2+ACO3=<br>0.50MO2+(1/3)*NQ2+(2/3)*NOQ+0.287<br>HCHO+1.24ALD+0.464KET+0.50ORA2 | 5.37E-13.*exp(765./T)  | 1 |
| R318c | OLNDQ3+ACO3=<br>0.50MO2+NQ2+0.287HCHO+1.24ALD+<br>0.464KET+0.50ORA2                 | 5.37E-13.*exp(765./T)  | 1 |
| R319  | ADCN+ACO3=HO2+MO2+0.7 NO2+0.7<br>GLY+0.7 OP2+0.3 ONIT                               | 7.40E-13.*exp(708./T)  | 1 |
| R319a | ADCNQ+ACO3=HO2+MO2+0.4667NOQ<br>+0.233NO2 + 0.7 GLY+0.7 OP2+0.3<br>ONITQ            | 7.40E-13.*exp(708./T)  | 1 |
| R319b | ADCNQ2+ACO3=HO2+MO2+0.4667NO<br>Q+0.233NQ2 + 0.7 GLY+0.7 OP2+0.3<br>ONITQ2          | 7.40E-13.*exp(708./T)  | 1 |
| R319c | ADCNQ3+ACO3=HO2+MO2+7NQ2 +<br>0.7 GLY+0.7 OP2+0.3 ONITQ3                            | 7.40E-13.*exp(708./T)  | 1 |
| R320  | XO2+ACO3=MO2  | 3.40E-14.*exp(1560./T) | 1 |

### Organic Peroxy Radical + NO<sub>3</sub>

|       |   |          |   |
|-------|---|----------|---|
| R321  | MO2+NO3=HCHO+HO2+NO2                      | 1.20E-12 | 1 |
| R321a | MO2+NO2Q=HCHO+HO2+(1/3)*NO2+(<br>2/3)*NOQ | 1.20E-12 | 1 |
| R321b | MO2+NOQ2=HCHO+HO2+(1/3)*NQ2+(<br>2/3)*NOQ | 1.20E-12 | 1 |
| R321c | MO2+NQ3=HCHO+HO2+NQ2                      | 1.20E-12 | 1 |
| R322  | ETHP+NO3=ACD+HO2+NO2                      | 1.20E-12 | 1 |
| R322a | ETHP+NO2Q=ACD+HO2+(1/3)*NO2+(2/<br>3)*NOQ | 1.20E-12 | 1 |
| R322b | ETHP+NOQ2=ACD+HO2+(1/3)*NQ2+(2/<br>3)*NOQ | 1.20E-12 | 1 |
| R322c | ETHP+NQ3=ACD+HO2+NQ2                      | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R323  | $\text{HC3P} + \text{NO}_3 = 0.254\text{HO}_2 + 0.140\text{MO}_2 + 0.095\text{ACT}$  | 1.20E-12 | 1 |
| R323a | $\text{HC3P} + \text{NO}_2\text{Q} = 0.254\text{HO}_2 + 0.140\text{MO}_2 + 0.092\text{XO}_2 + 0.503\text{ETHP} + \text{NO}_2 + 0.519\text{ACD} + 0.147\text{ALD} + 0.075\text{MEK} + 0.095\text{ACT}$  | 1.20E-12 | 1 |
| R323b | $\text{HC3P} + \text{NOQ}_2 = 0.254\text{HO}_2 + 0.140\text{MO}_2 + 0.092\text{XO}_2 + 0.503\text{ETHP} + (1/3)\text{NO}_2 + (2/3)\text{NOQ} + 0.519\text{ACD} + 0.147\text{ALD} + 0.075\text{MEK} + 0.095\text{ACT}$  | 1.20E-12 | 1 |
| R323c | $\text{HC3P} + \text{NQ}_3 = 0.254\text{HO}_2 + 0.140\text{MO}_2 + 0.092\text{XO}_2 + 0.503\text{ETHP} + \text{NQ}_2 + 0.519\text{ACD} + 0.147\text{ALD} + 0.075\text{MEK} + 0.095\text{ACT}$  | 1.20E-12 | 1 |
| R324  | $\text{HC5P} + \text{NO}_3 = 0.488\text{HO}_2 + 0.055\text{MO}_2 + 0.28\text{ETHP} + 0.485\text{XO}_2 + \text{NO}_2 + 0.024\text{HCHO} + 0.241\text{ALD} + 0.06\text{KET} + 0.063\text{MEK} + 0.247\text{ACT} + 0.048\text{ACD} + 0.275\text{HKET}$                                | 1.20E-12 | 1 |
| R324a | $\text{HC5P} + \text{NO}_2\text{Q} = 0.488\text{HO}_2 + 0.055\text{MO}_2 + 0.28\text{ETHP} + 0.485\text{XO}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + 0.024\text{HCHO} + 0.241\text{ALD} + 0.06\text{KET} + 0.063\text{MEK} + 0.247\text{ACT} + 0.048\text{ACD} + 0.275\text{HKET}$ | 1.20E-12 | 1 |
| R324b | $\text{HC5P} + \text{NOQ}_2 = 0.488\text{HO}_2 + 0.055\text{MO}_2 + 0.28\text{ETHP} + 0.485\text{XO}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + 0.024\text{HCHO} + 0.241\text{ALD} + 0.06\text{KET} + 0.063\text{MEK} + 0.247\text{ACT} + 0.048\text{ACD} + 0.275\text{HKET}$        | 1.20E-12 | 1 |
| R324c | $\text{HC5P} + \text{NQ}_3 = 0.488\text{HO}_2 + 0.055\text{MO}_2 + 0.28\text{ETHP} + 0.485\text{XO}_2 + \text{NQ}_2 + 0.024\text{HCHO} + 0.241\text{ALD} + 0.06\text{KET} + 0.063\text{MEK} + 0.247\text{ACT} + 0.048\text{ACD} + 0.275\text{HKET}$                                | 1.20E-12 | 1 |
| R325  | $\text{HC8P} + \text{NO}_3 = 0.82\text{HO}_2 + 0.18\text{ETHP} + 0.563\text{XO}_2 + \text{NO}_2 + 0.203\text{ALD} + 0.869\text{KET}$   | 1.20E-12 | 1 |
| R325a | $\text{HC8P} + \text{NO}_2\text{Q} = 0.82\text{HO}_2 + 0.18\text{ETHP} + 0.563\text{XO}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + 0.203\text{ALD} + 0.869\text{KET}$  | 1.20E-12 | 1 |
| R325b | $\text{HC8P} + \text{NOQ}_2 = 0.82\text{HO}_2 + 0.18\text{ETHP} + 0.563\text{XO}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + 0.203\text{ALD} + 0.869\text{KET}$   | 1.20E-12 | 1 |
| R325c | $\text{HC8P} + \text{NQ}_3 = 0.82\text{HO}_2 + 0.18\text{ETHP} + 0.563\text{XO}_2 + \text{NQ}_2 + 0.203\text{ALD} + 0.869\text{KET}$   | 1.20E-12 | 1 |
| R326  | $\text{ETEP} + \text{NO}_3 = \text{HO}_2 + \text{NO}_2 + 1.6\text{ HCHO} + 0.2\text{ ALD}$   | 1.20E-12 | 1 |

|       |   |          |   |
|-------|---|----------|---|
| R326a | ETEP+NO2Q=HO2+(2/3)NOQ+(1/3)NO2 +1.6 HCHO+0.2 ALD                                       | 1.20E-12 | 1 |
| R326b | ETEP+NOQ2=HO2+(2/3)NOQ+(1/3)NQ2 +1.6 HCHO+0.2 ALD                                       | 1.20E-12 | 1 |
| R326c | ETEP+NQ3=HO2+NQ2+1.6 HCHO+0.2 ALD   | 1.20E-12 | 1 |
| R327  | OLTP+NO3= 0.47ALD + HCHO + 0.79HO2 + NO2 + 0.18MEK + 0.02ACD + 0.09ACT                  | 1.20E-12 | 1 |
| R327a | OLTP+NO2Q= 0.47ALD + HCHO + 0.79HO2+(2/3)NOQ+(1/3)NO2+ 0.18MEK + 0.02ACD + 0.09ACT      | 1.20E-12 | 1 |
| R327b | OLTP+NOQ2= 0.47ALD + HCHO + 0.79HO2+(2/3)NOQ+(1/3)NQ2+ 0.18MEK + 0.02ACD + 0.09ACT      | 1.20E-12 | 1 |
| R327c | OLTP+NQ3= 0.47ALD + HCHO + 0.79HO2+NQ2+ 0.18MEK + 0.02ACD + 0.09ACT                     | 1.20E-12 | 1 |
| R328  | OLIP+NO3= 0.86HO2 + 0.72ALD + 0.11KET + NO2 + 0.20ACT + 0.85ACD + 0.04HKET              | 1.20E-12 | 1 |
| R328a | OLIP+NO2Q= 0.86HO2 + 0.72ALD + 0.11KET +(2/3)NOQ+(1/3)NO2+ 0.20ACT + 0.85ACD + 0.04HKET | 1.20E-12 | 1 |
| R328b | OLIP+NOQ2= 0.86HO2 + 0.72ALD + 0.11KET +(2/3)NOQ+(1/3)NQ2+ 0.20ACT + 0.85ACD + 0.04HKET | 1.20E-12 | 1 |
| R328c | OLIP+NQ3= 0.86HO2 + 0.72ALD + 0.11KET +NQ2+ 0.20ACT + 0.85ACD + 0.04HKET                | 1.20E-12 | 1 |
| R329  | BENP+NO3=HO2+GLY+0.5DCB2+NO2+ 0.5DCB3   | 1.20E-12 | 1 |
| R329a | BENP+NO2Q=HO2+GLY+0.5DCB2+(2/3 )NOQ+(1/3)NO2+0.5DCB3                                    | 1.20E-12 | 1 |
| R329b | BENP+NOQ2=HO2+GLY+0.5DCB2+(2/3 )NOQ+(1/3)NQ2+0.5DCB3                                    | 1.20E-12 | 1 |
| R329c | BENP+NQ3=HO2+GLY+0.5DCB2+NQ2+ 0.5DCB3   | 1.20E-12 | 1 |
| R330  | TLP1+NO3=NO2+BALD   | 1.20E-12 | 1 |
| R330a | TLP1+NO2Q=(2/3)NOQ+(1/3)NO2+BAL D   | 1.20E-12 | 1 |
| R330b | TLP1+NOQ2=(2/3)NOQ+(1/3)NQ2+BAL D   | 1.20E-12 | 1 |
| R330c | TLP1+NQ3=NQ2+BALD   | 1.20E-12 | 1 |
| R331  | TOLP+NO3=DCB2+NO2+HO2   | 1.20E-12 | 1 |
| R331a | TOLP+NO2Q=DCB2+(2/3)NOQ+(1/3)NO 2+HO2   | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R331b | TOLP+NOQ2=DCB2+(2/3)NOQ+(1/3)NQ<br>2+HO2   | 1.20E-12 | 1 |
| R331c | TOLP+NQ3=DCB2+NQ2+HO2  | 1.20E-12 | 1 |
| R332  | PER1+NO3=0.5DCB1+NO2+0.5MGLY+0<br>.5HO2+0.5BALD  | 1.20E-12 | 1 |
| R332a | PER1+NO2Q=0.5DCB1+(2/3)NOQ+(1/3)<br>NO2+0.5MGLY+0.5HO2+0.5BALD                               | 1.20E-12 | 1 |
| R332b | PER1+NOQ2=0.5DCB1+(2/3)NOQ+(1/3)<br>NQ2+0.5MGLY+0.5HO2+0.5BALD                               | 1.20E-12 | 1 |
| R332c | PER1+NQ3=0.5DCB1+NQ2+0.5MGLY+0<br>.5HO2+0.5BALD  | 1.20E-12 | 1 |
| R333  | XYL1+NO3=NO2+BALD  | 1.20E-12 | 1 |
| R333a | XYL1+NO2Q=(2/3)NOQ+(1/3)NO2+BAL<br>D   | 1.20E-12 | 1 |
| R333b | XYL1+NOQ2=(2/3)NOQ+(1/3)NQ2+BAL<br>D   | 1.20E-12 | 1 |
| R333c | XYL1+NQ3=NQ2+BALD  | 1.20E-12 | 1 |
| R334  | XYLP+NO3=DCB3+NO2+HO2  | 1.20E-12 | 1 |
| R334a | XYLP+NO2Q=DCB3+(2/3)NOQ+(1/3)NO<br>2+HO2   | 1.20E-12 | 1 |
| R334b | XYLP+NOQ2=DCB3+(2/3)NOQ+(1/3)NQ<br>2+HO2   | 1.20E-12 | 1 |
| R334c | XYLP+NQ3=DCB3+NQ2+HO2  | 1.20E-12 | 1 |
| R335  | PER2+NO3=DCB1+NO2+MGLY+HO2+1.<br>05DCB3  | 1.20E-12 | 1 |
| R335a | PER2+NO2Q=DCB1+(2/3)NOQ+(1/3)NO<br>2+MGLY+HO2+1.05DCB3                                       | 1.20E-12 | 1 |
| R335b | PER2+NOQ2=DCB1+(2/3)NOQ+(1/3)NQ<br>2+MGLY+HO2+1.05DCB3                                       | 1.20E-12 | 1 |
| R335c | PER2+NQ3=DCB1+NQ2+MGLY+HO2+1.<br>05DCB3  | 1.20E-12 | 1 |
| R336  | XYOP+NO3=HO2+NO2+0.368<br>GLY+0.632 MGLY+0.737 DCB1+0.077<br>DCB2+0.186 DCB3                 | 1.20E-12 | 1 |
| R336a | XYOP+NO2Q=HO2+(2/3)NOQ+(1/3)NO<br>2+0.368 GLY+0.632 MGLY+0.737<br>DCB1+0.077 DCB2+0.186 DCB3 | 1.20E-12 | 1 |
| R336b | XYOP+NOQ2=HO2+(2/3)NOQ+(1/3)NQ<br>2+0.368 GLY+0.632 MGLY+0.737<br>DCB1+0.077 DCB2+0.186 DCB3 | 1.20E-12 | 1 |
| R336c | XYOP+NQ3=HO2+NQ2+0.368<br>GLY+0.632 MGLY+0.737 DCB1+0.077<br>DCB2+0.186 DCB3                 | 1.20E-12 | 1 |
| R337  | ISOP+NO3=HO2 + NO2 + 0.75HCHO +<br>0.318MACR + 0.5MVK + 0.024GLY +<br>0.033HKET + 0.031ALD   | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R337a | $\text{ISOP} + \text{NO}_2\text{Q} = \text{HO}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + 0.75\text{HCHO} + 0.318\text{MACR} + 0.5\text{MVK} + 0.024\text{GLY} + 0.033\text{HKET} + 0.031\text{ALD}$ | 1.20E-12 | 1 |
| R337b | $\text{ISOP} + \text{NOQ}_2 = \text{HO}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + 0.75\text{HCHO} + 0.318\text{MACR} + 0.5\text{MVK} + 0.024\text{GLY} + 0.033\text{HKET} + 0.031\text{ALD}$        | 1.20E-12 | 1 |
| R337c | $\text{ISOP} + \text{NQ}_3 = \text{HO}_2 + \text{NQ}_2 + 0.75\text{HCHO} + 0.318\text{MACR} + 0.5\text{MVK} + 0.024\text{GLY} + 0.033\text{HKET} + 0.031\text{ALD}$                                | 1.20E-12 | 1 |
| R338  | $\text{APIP} + \text{NO}_3 = \text{HO}_2 + \text{ALD} + \text{NO}_2 + \text{KET}$  | 1.20E-12 | 1 |
| R338a | $\text{APIP} + \text{NO}_2\text{Q} = \text{HO}_2 + \text{ALD} + (1/3)*\text{NO}_2 + (2/3)*\text{NOQ} + \text{KET}$   | 1.20E-12 | 1 |
| R338b | $\text{APIP} + \text{NOQ}_2 = \text{HO}_2 + \text{ALD} + (1/3)*\text{NQ}_2 + (2/3)*\text{NOQ} + \text{KET}$  | 1.20E-12 | 1 |
| R338c | $\text{APIP} + \text{NQ}_3 = \text{HO}_2 + \text{ALD} + \text{NQ}_2 + \text{KET}$  | 1.20E-12 | 1 |
| R339  | $\text{LIMP} + \text{NO}_3 = \text{HO}_2 + \text{NO}_2 + 0.385 \text{OLI} + 0.385 \text{HCHO} + 0.615 \text{MACR}$   | 1.20E-12 | 1 |
| R339a | $\text{LIMP} + \text{NO}_2\text{Q} = \text{HO}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + 0.385 \text{OLI} + 0.385 \text{HCHO} + 0.615 \text{MACR}$  | 1.20E-12 | 1 |
| R339b | $\text{LIMP} + \text{NOQ}_2 = \text{HO}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + 0.385 \text{OLI} + 0.385 \text{HCHO} + 0.615 \text{MACR}$   | 1.20E-12 | 1 |
| R339c | $\text{LIMP} + \text{NQ}_3 = \text{HO}_2 + \text{NQ}_2 + 0.385 \text{OLI} + 0.385 \text{HCHO} + 0.615 \text{MACR}$   | 1.20E-12 | 1 |
| R340  | $\text{ACO}_3 + \text{NO}_3 = \text{MO}_2 + \text{NO}_2$   | 4.00E-12 | 1 |
| R340a | $\text{ACO}_3 + \text{NO}_2\text{Q} = \text{MO}_2 + (1/3)*\text{NO}_2 + (2/3)*\text{NOQ}$  | 4.00E-12 | 1 |
| R340b | $\text{ACO}_3 + \text{NOQ}_2 = \text{MO}_2 + (1/3)*\text{NQ}_2 + (2/3)*\text{NOQ}$   | 4.00E-12 | 1 |
| R340c | $\text{ACO}_3 + \text{NQ}_3 = \text{MO}_2 + \text{NQ}_2$   | 4.00E-12 | 1 |
| R341  | $\text{RCO}_3 + \text{NO}_3 = \text{ETHP} + \text{NO}_2$   | 4.00E-12 | 1 |
| R341a | $\text{RCO}_3 + \text{NO}_2\text{Q} = \text{ETHP} + (1/3)*\text{NO}_2 + (2/3)*\text{NOQ}$  | 4.00E-12 | 1 |
| R341b | $\text{RCO}_3 + \text{NOQ}_2 = \text{ETHP} + (1/3)*\text{NQ}_2 + (2/3)*\text{NOQ}$   | 4.00E-12 | 1 |
| R341c | $\text{RCO}_3 + \text{NQ}_3 = \text{ETHP} + \text{NQ}_2$   | 4.00E-12 | 1 |
| R342  | $\text{ACTP} + \text{NO}_3 = \text{ACO}_3 + \text{NO}_2 + \text{HCHO}$   | 1.20E-12 | 1 |
| R342a | $\text{ACTP} + \text{NO}_2\text{Q} = \text{ACO}_3 + (1/3)*\text{NO}_2 + (2/3)*\text{NOQ} + \text{HCHO}$  | 1.20E-12 | 1 |
| R342b | $\text{ACTP} + \text{NOQ}_2 = \text{ACO}_3 + (1/3)*\text{NQ}_2 + (2/3)*\text{NOQ} + \text{HCHO}$   | 1.20E-12 | 1 |
| R342c | $\text{ACTP} + \text{NQ}_3 = \text{ACO}_3 + \text{NQ}_2\text{HCHO}$  | 1.20E-12 | 1 |
| R343  | $\text{MEKP} + \text{NO}_3 = 0.67 \text{HO}_2 + \text{NO}_2 + 0.33 \text{HCHO} + 0.67 \text{DCB}_1$  | 1.20E-12 | 1 |
| R343a | $\text{MEKP} + \text{NO}_2\text{Q} = 0.67 \text{HO}_2 + (1/3)*\text{NO}_2 + (2/3)*\text{NOQ} + 0.33 \text{HCHO} + 0.67 \text{DCB}_1$   | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R343b | MEKP+NOQ2=0.67<br>HO2+(1/3)*NQ2+(2/3)*NOQ+0.33<br>HCHO+0.67 DCB1                             | 1.20E-12 | 1 |
| R343c | MEKP+NQ3=0.67 HO2+NQ2+0.33<br>HCHO+0.67 DCB1   | 1.20E-12 | 1 |
| R344  | KETP+NO3=DCB1+HO2+NO2  | 1.20E-12 | 1 |
| R344a | KETP+NO2Q=DCB1+HO2+(1/3)*NO2+(<br>2/3)*NOQ   | 1.20E-12 | 1 |
| R344b | KETP+NOQ2=DCB1+HO2+(1/3)*NQ2+(<br>2/3)*NOQ   | 1.20E-12 | 1 |
| R344c | KETP+NQ3=DCB1+HO2+NQ2  | 1.20E-12 | 1 |
| R345  | MACP+NO3=HO2+0.33<br>ACO3+NO2+0.33 CO+HCHO+0.33<br>HKET+0.667 MGLY                           | 1.20E-12 | 1 |
| R345a | MACP+NO2Q=HO2+0.33<br>ACO3+(2/3)NOQ+(1/3)NO2+0.33<br>CO+HCHO+0.33 HKET+0.667 MGLY            | 1.20E-12 | 1 |
| R345b | MACP+NOQ2=HO2+0.33<br>ACO3+(2/3)NOQ+(1/3)NQ2+0.33<br>CO+HCHO+0.33 HKET+0.667 MGLY            | 1.20E-12 | 1 |
| R345c | MACP+NQ3=HO2+0.33<br>ACO3+NQ2+0.33 CO+HCHO+0.33<br>HKET+0.667 MGLY                           | 1.20E-12 | 1 |
| R346  | MCP+NO3 = NO2+HO2+HCHO+HKET  | 1.20E-12 | 1 |
| R346a | MCP+NO2Q =<br>(2/3)NOQ+(1/3)NO2+HO2+HCHO+HKE<br>T  | 1.20E-12 | 1 |
| R346b | MCP+NOQ2 =<br>(2/3)NOQ+(1/3)NQ2+HO2+HCHO+HKE<br>T  | 1.20E-12 | 1 |
| R346c | MCP+NQ3 = NQ2+HO2+HCHO+HKET  | 1.20E-12 | 1 |
| R347  | MVKP+NO3=0.3 HO2+0.7 ACO3+0.7<br>XO2+NO2+0.3 HCHO+0.7 ALD+MGLY                               | 1.20E-12 | 1 |
| R347a | MVKP+NO2Q=0.3 HO2+0.7 ACO3+0.7<br>XO2+(2/3)NOQ+(1/3)NO2+0.3<br>HCHO+0.7 ALD+MGLY             | 1.20E-12 | 1 |
| R347b | MVKP+NOQ2=0.3 HO2+0.7 ACO3+0.7<br>XO2+(2/3)NOQ+(1/3)NQ2+0.3<br>HCHO+0.7 ALD+MGLY             | 1.20E-12 | 1 |
| R347c | MVKP+NQ3=0.3 HO2+0.7 ACO3+0.7<br>XO2+NQ2+0.3 HCHO+0.7 ALD+MGLY                               | 1.20E-12 | 1 |
| R348  | UALP+NO3=HO2+NO2+0.61 CO+0.03<br>HCHO+0.27 ALD+0.7 KET+0.18<br>GLY+0.21 MGLY                 | 1.20E-12 | 1 |
| R348a | UALP+NO2Q=HO2+(2/3)NOQ+(1/3)NO<br>2+0.61 CO+0.03 HCHO+0.27 ALD+0.7<br>KET+0.18 GLY+0.21 MGLY | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R348b | $UALP + NOQ_2 = HO_2 + (2/3)NOQ + (1/3)NQ$<br>2+0.61 CO+0.03 HCHO+0.27 ALD+0.7<br>KET+0.18 GLY+0.21 MGLY | 1.20E-12 | 1 |
| R348c | $UALP + NQ_3 = HO_2 + NQ_2 + 0.61 CO + 0.03$<br>HCHO+0.27 ALD+0.7 KET+0.18<br>GLY+0.21 MGLY              | 1.20E-12 | 1 |
| R349  | $BALP + NO_3 = BAL_1 + NO_2$   | 1.20E-12 | 1 |
| R349a | $BALP + NO_2 Q = BAL_1 + (2/3)NOQ + (1/3)NO$<br>2  | 1.20E-12 | 1 |
| R349b | $BALP + NOQ_2 = BAL_1 + (2/3)NOQ + (1/3)NQ$<br>2   | 1.20E-12 | 1 |
| R349c | $BALP + NQ_3 = BAL_1 + NQ_2$   | 1.20E-12 | 1 |
| R350  | $BAL_1 + NO_3 = BAL_2 + NO_2$  | 1.20E-12 | 1 |
| R350a | $BAL_1 + NO_2 Q = BAL_2 + (2/3)NOQ + (1/3)NO$<br>2   | 1.20E-12 | 1 |
| R350b | $BAL_1 + NOQ_2 = BAL_2 + (2/3)NOQ + (1/3)NQ$<br>2  | 1.20E-12 | 1 |
| R350c | $BAL_1 + NQ_3 = BAL_2 + NQ_2$  | 1.20E-12 | 1 |
| R351  | $ADD C + NO_3 = HO_2 + NO_2 + 0.32$<br>HKET+0.68 GLY+0.68 OP2  | 1.20E-12 | 1 |
| R351a | $ADD C + NO_2 Q = HO_2 + (2/3)NOQ + (1/3)NO$<br>2+0.32 HKET+0.68 GLY+0.68 OP2                            | 1.20E-12 | 1 |
| R351b | $ADD C + NOQ_2 = HO_2 + (2/3)NOQ + (1/3)NQ$<br>2+0.32 HKET+0.68 GLY+0.68 OP2                             | 1.20E-12 | 1 |
| R351c | $ADD C + NQ_3 = HO_2 + NQ_2 + 0.32$<br>HKET+0.68 GLY+0.68 OP2  | 1.20E-12 | 1 |
| R352  | $MCTP + NO_3 = MCTO + NO_2$  | 1.20E-12 | 1 |
| R352a | $MCTP + NO_2 Q = MCTO + (2/3)NOQ + (1/3)NO$<br>2   | 1.20E-12 | 1 |
| R352b | $MCTP + NOQ_2 = MCTO + (2/3)NOQ + (1/3)NQ$<br>2  | 1.20E-12 | 1 |
| R352c | $MCTP + NQ_3 = MCTO + NQ_2$  | 1.20E-12 | 1 |
| R353  | $ORAP + NO_3 = HO_2 + NO_2 + GLY$  | 1.20E-12 | 1 |
| R353a | $ORAP + NO_2 Q = HO_2 + (1/3)*NO_2 + (2/3)*NO$<br>Q+GLY  | 1.20E-12 | 1 |
| R353b | $ORAP + NOQ_2 = HO_2 + (1/3)*NQ_2 + (2/3)*NO$<br>Q+GLY   | 1.20E-12 | 1 |
| R353c | $ORAP + NQ_3 = HO_2 + NQ_2 + GLY$  | 1.20E-12 | 1 |
| R354  | $OLNN + NO_3 = ONIT + NO_2 + HO_2$   | 1.20E-12 | 1 |
| R354a | $OLNN + NO_2 Q = ONIT + (1/3)*NO_2 + (2/3)*NO$<br>Q+HO2  | 1.20E-12 | 1 |
| R354b | $OLNN + NOQ_2 = ONIT + (1/3)*NQ_2 + (2/3)*NO$<br>Q+HO2   | 1.20E-12 | 1 |
| R354c | $OLNN + NQ_3 = ONIT + NQ_2 + HO_2$   | 1.20E-12 | 1 |
| R354d | $OLNNQ + NO_3 = ONITQ + NO_2 + HO_2$   | 1.20E-12 | 1 |
| R354e | $OLNNQ + NO_2 Q = ONITQ + (1/3)*NO_2 + (2/3)*NO$<br>Q+HO2  | 1.20E-12 | 1 |

|       |  |          |   |
|-------|--|----------|---|
| R354f | $\text{OLNNQ} + \text{NOQ}_2 = \text{ONITQ} + (1/3) * \text{NQ}_2 + (2/3) * \text{NOQ} + \text{HO}_2$                                    | 1.20E-12 | 1 |
| R354g | $\text{OLNNQ} + \text{NQ}_3 = \text{ONITQ} + \text{NQ}_2 + \text{HO}_2$  | 1.20E-12 | 1 |
| R354h | $\text{OLNNQ}_2 + \text{NO}_3 = \text{ONITQ}_2 + \text{NO}_2 + \text{HO}_2$  | 1.20E-12 | 1 |
| R354i | $\text{OLNNQ}_2 + \text{NO}_2\text{Q} = \text{ONITQ}_2 + (1/3) * \text{NO}_2 + (2/3) * \text{NOQ} + \text{HO}_2$                         | 1.20E-12 | 1 |
| R354j | $\text{OLNNQ}_2 + \text{NOQ}_2 = \text{ONITQ}_2 + (1/3) * \text{NQ}_2 + (2/3) * \text{NOQ} + \text{HO}_2$                                | 1.20E-12 | 1 |
| R354k | $\text{OLNNQ}_2 + \text{NQ}_3 = \text{ONITQ}_2 + \text{NQ}_2 + \text{HO}_2$  | 1.20E-12 | 1 |
| R354l | $\text{OLNNQ}_3 + \text{NO}_3 = \text{ONITQ}_3 + \text{NO}_2 + \text{HO}_2$  | 1.20E-12 | 1 |
| R354m | $\text{OLNNQ}_3 + \text{NO}_2\text{Q} = \text{ONITQ}_3 + (1/3) * \text{NO}_2 + (2/3) * \text{NOQ} + \text{HO}_2$                         | 1.20E-12 | 1 |
| R354n | $\text{OLNNQ}_3 + \text{NOQ}_2 = \text{ONITQ}_3 + (1/3) * \text{NQ}_2 + (2/3) * \text{NOQ} + \text{HO}_2$                                | 1.20E-12 | 1 |
| R354o | $\text{OLNNQ}_3 + \text{NQ}_3 = \text{ONITQ}_3 + \text{NQ}_2 + \text{HO}_2$  | 1.20E-12 | 1 |
| R355  | $\text{OLND} + \text{NO}_3 = 2 \text{NO}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                                     | 1.20E-12 | 1 |
| R355a | $\text{OLND} + \text{NO}_2\text{Q} = \text{NO}_2 + \text{NOQ} + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                  | 1.20E-12 | 1 |
| R355b | $\text{OLND} + \text{NOQ}_2 = \text{NO}_2 + \text{NOQ} + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                         | 1.20E-12 | 1 |
| R355c | $\text{OLND} + \text{NQ}_3 = \text{NO}_2 + \text{NOQ} + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                          | 1.20E-12 | 1 |
| R355d | $\text{OLNDQ} + \text{NO}_3 = \text{NO}_2 + \text{NOQ} + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                         | 1.20E-12 | 1 |
| R355e | $\text{OLNDQ} + \text{NO}_2\text{Q} = \text{NO}_2 + \text{NOQ} + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                 | 1.20E-12 | 1 |
| R355f | $\text{OLNDQ} + \text{NOQ}_2 = \text{NO}_2 + \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$          | 1.20E-12 | 1 |
| R355g | $\text{OLNDQ} + \text{NQ}_3 = \text{NO}_2 + \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$           | 1.20E-12 | 1 |
| R355h | $\text{OLNDQ}_2 + \text{NO}_3 = \text{NO}_2 + \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$         | 1.20E-12 | 1 |
| R355i | $\text{OLNDQ}_2 + \text{NO}_2\text{Q} = \text{NO}_2 + \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$ | 1.20E-12 | 1 |
| R355j | $\text{OLNDQ}_2 + \text{NOQ}_2 = \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                      | 1.20E-12 | 1 |
| R355k | $\text{OLNDQ}_2 + \text{NQ}_3 = \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                       | 1.20E-12 | 1 |
| R355l | $\text{OLNDQ}_3 + \text{NO}_3 = \text{NO}_2 + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                      | 1.20E-12 | 1 |
| R355m | $\text{OLNDQ}_3 + \text{NO}_2\text{Q} = \text{NO}_2 + \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$ | 1.20E-12 | 1 |
| R355n | $\text{OLNDQ}_3 + \text{NOQ}_2 = \text{NOQ} + \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                      | 1.20E-12 | 1 |
| R355o | $\text{OLNDQ}_3 + \text{NQ}_3 = \text{NQ}_2 + 0.287 \text{HCHO} + 1.24 \text{ALD} + 0.464 \text{KET}$                                    | 1.20E-12 | 1 |

|       |   |          |   |
|-------|---|----------|---|
| R356  | $\text{ADCN} + \text{NO}_3 = \text{OP}_2 + \text{GLY} + \text{NO}_2 + \text{NO}_2$  | 1.20E-12 | 1 |
| R356a | $\text{ADCN} + \text{NO}_2\text{Q} = \text{OP}_2 + \text{GLY} + \text{NO}_2 + (2/3)\text{NO}$<br>$\text{Q} + (1/3)\text{NO}_2$              | 1.20E-12 | 1 |
| R356b | $\text{ADCN} + \text{NOQ}_2 = \text{OP}_2 + \text{GLY} + \text{NO}_2 + (2/3)\text{NO}$<br>$\text{Q} + (1/3)\text{NQ}_2$                     | 1.20E-12 | 1 |
| R356c | $\text{ADCN} + \text{NQ}_3 = \text{OP}_2 + \text{GLY} + \text{NO}_2 + \text{NQ}_2$  | 1.20E-12 | 1 |
| R356d | $\text{ADCNQ} + \text{NO}_3 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + \text{NO}_2$                                  | 1.20E-12 | 1 |
| R356e | $\text{ADCNQ} + \text{NO}_2\text{Q} = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2$   | 1.20E-12 | 1 |
| R356f | $\text{ADCNQ} + \text{NOQ}_2 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2$          | 1.20E-12 | 1 |
| R356g | $\text{ADCNQ} + \text{NQ}_3 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NO}_2 + \text{NQ}_2$                                  | 1.20E-12 | 1 |
| R356h | $\text{ADCNQ}_2 + \text{NO}_3 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + \text{NO}_2$                                | 1.20E-12 | 1 |
| R356i | $\text{ADCNQ}_2 + \text{NO}_2\text{Q} = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2$ | 1.20E-12 | 1 |
| R356j | $\text{ADCNQ}_2 + \text{NOQ}_2 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2$        | 1.20E-12 | 1 |
| R356k | $\text{ADCNQ}_2 + \text{NQ}_3 = \text{OP}_2 + \text{GLY} + (2/3)\text{NOQ} + (1/3)\text{NQ}_2 + \text{NQ}_2$                                | 1.20E-12 | 1 |
| R356l | $\text{ADCNQ}_3 + \text{NO}_3 = \text{OP}_2 + \text{GLY} + \text{NQ}_2 + \text{NO}_2$   | 1.20E-12 | 1 |
| R356m | $\text{ADCNQ}_3 + \text{NO}_2\text{Q} = \text{OP}_2 + \text{GLY} + \text{NQ}_2 + (2/3)\text{NOQ} + (1/3)\text{NO}_2$                        | 1.20E-12 | 1 |
| R356n | $\text{ADCNQ}_3 + \text{NOQ}_2 = \text{OP}_2 + \text{GLY} + \text{NQ}_2 + (2/3)\text{NOQ} + (1/3)\text{NQ}_2$                               | 1.20E-12 | 1 |
| R356o | $\text{ADCNQ}_3 + \text{NQ}_3 = \text{OP}_2 + \text{GLY} + \text{NQ}_2 + \text{NQ}_2$   | 1.20E-12 | 1 |
| R357  | $\text{XO}_2 + \text{NO}_3 = \text{NO}_2$   | 1.20E-12 | 1 |
| R357a | $\text{XO}_2 + \text{NO}_2\text{Q} = (1/3)*\text{NO}_2 + (2/3)*\text{NOQ}$  | 1.20E-12 | 1 |
| R357b | $\text{XO}_2 + \text{NOQ}_2 = (1/3)*\text{NQ}_2 + (2/3)*\text{NOQ}$   | 1.20E-12 | 1 |
| R357c | $\text{XO}_2 + \text{NQ}_3 = \text{NQ}_2$   | 1.20E-12 | 1 |

#### Self-Reaction of $\text{RCO}_3$ Radical

|       |   |                                   |   |
|-------|---|-----------------------------------|---|
| R358  | $\text{RCO}_3 + \text{RCO}_3 = 2\text{ETHP} + 2\text{CO}_2$                       | $2.5\text{e-12} * \exp(500./T)$   | 1 |
| R359  | $\text{OLNN} + \text{OLNN} = \text{ONIT} + \text{ONIT} + \text{HO}_2$             | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359a | $\text{OLNN} + \text{OLNNQ} = \text{ONIT} + \text{ONITQ} + \text{HO}_2$           | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359b | $\text{OLNN} + \text{OLNNQ}_2 = \text{ONIT} + \text{ONITQ}_2 + \text{HO}_2$       | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359c | $\text{OLNN} + \text{OLNNQ}_3 = \text{ONIT} + \text{ONITQ}_3 + \text{HO}_2$       | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359d | $\text{OLNNQ} + \text{OLNNQ} = \text{ONITQ} + \text{ONITQ} + \text{HO}_2$         | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359e | $\text{OLNNQ} + \text{OLNNQ}_2 = \text{ONITQ} + \text{ONITQ}_2 + \text{HO}_2$     | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359f | $\text{OLNNQ} + \text{OLNNQ}_3 = \text{ONITQ} + \text{ONITQ}_3 + \text{HO}_2$     | $7.00\text{E-14} * \exp(1000./T)$ | 1 |
| R359g | $\text{OLNNQ}_2 + \text{OLNNQ}_2 = \text{ONITQ}_2 + \text{ONITQ}_2 + \text{HO}_2$ | $7.00\text{E-14} * \exp(1000./T)$ | 1 |

|       |  |                        |   |
|-------|--|------------------------|---|
| R359h | OLNNQ2+OLNNQ3=ONITQ2+ONITQ3+HO2  | 7.00E-14.*exp(1000./T) | 1 |
| R359i | OLNNQ3+OLNNQ3=ONITQ3+ONITQ3+HO2  | 7.00E-14.*exp(1000./T) | 1 |
| R360  | OLNN+OLND=0.50 HO2+0.50 NO2+0.202 HCHO+0.640 ALD+0.149 KET+1.50 ONIT         | 4.25E-14.*exp(1000./T) | 1 |
| R360a | OLNN+OLNDQ=0.50 HO2+NO2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONIT +ONITQ      | 4.25E-14.*exp(1000./T) | 1 |
| R360b | OLNN+OLNDQ2=0.50 HO2+NQ2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONIT +ONITQ2    | 4.25E-14.*exp(1000./T) | 1 |
| R360c | OLNN+OLNDQ3=0.50 HO2+NQ2+0.202 HCHO+0.640 ALD+0.149 KET+ ONIT +ONITQ3        | 4.25E-14.*exp(1000./T) | 1 |
| R360d | OLNNQ+OLND=0.50 HO2+NO2+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ +ONIT          | 4.25E-14.*exp(1000./T) | 1 |
| R360e | OLNNQ+OLNDQ=0.50 HO2+NO2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ           | 4.25E-14.*exp(1000./T) | 1 |
| R360f | OLNNQ+OLNDQ2=0.50 HO2+NQ2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ+ONITQ2   | 4.25E-14.*exp(1000./T) | 1 |
| R360g | OLNNQ+OLNDQ3=0.50 HO2+NQ2+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ+ONITQ3       | 4.25E-14.*exp(1000./T) | 1 |
| R360h | OLNNQ2+OLND=0.50 HO2+NO2+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ2+ONIT         | 4.25E-14.*exp(1000./T) | 1 |
| R360i | OLNNQ2+OLNDQ=0.50 HO2+NO2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ2+ONITQ   | 4.25E-14.*exp(1000./T) | 1 |
| R360j | OLNNQ2+OLNDQ2=0.50 HO2+NQ2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ2+ONITQ2 | 4.25E-14.*exp(1000./T) | 1 |
| R360k | OLNNQ2+OLNDQ3=0.50 HO2+NQ2+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ2+ONITQ3     | 4.25E-14.*exp(1000./T) | 1 |
| R360l | OLNNQ3+OLND=0.50 HO2+NO2+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ3+ONIT         | 4.25E-14.*exp(1000./T) | 1 |
| R360m | OLNNQ3+OLNDQ=0.50 HO2+NO2+NOQ+0.202 HCHO+0.640 ALD+0.149 KET+ ONITQ3+ONITQ   | 4.25E-14.*exp(1000./T) | 1 |

|       |  |                        |   |
|-------|--|------------------------|---|
| R360n | OLNNQ3+OLNDQ2=0.50<br>HO2+NQ2+NOQ+0.202 HCHO+0.640<br>ALD+0.149 KET+ ONITQ3+ONITQ2 | 4.25E-14.*exp(1000./T) | 1 |
| R360o | OLNNQ3+OLNDQ3=0.50<br>HO2+NQ2+0.202 HCHO+0.640<br>ALD+0.149 KET+ ONITQ3            | 4.25E-14.*exp(1000./T) | 1 |
| R361  | OLND+OLND=NO2+0.504 HCHO+1.21<br>ALD+0.285 KET+ONIT                                | 2.96E-14.*exp(1000./T) | 1 |
| R361a | OLND+OLNDQ=NO2+NOQ+0.504<br>HCHO+1.21 ALD+0.285<br>KET+ONIT+ONITQ                  | 2.96E-14.*exp(1000./T) | 1 |
| R361b | OLND+OLNDQ2=NO2+NOQ+NQ2+0.50<br>4 HCHO+1.21 ALD+0.285<br>KET+ONIT+ONITQ2           | 2.96E-14.*exp(1000./T) | 1 |
| R361c | OLND+OLNDQ3=NO2+NQ2+0.504<br>HCHO+1.21 ALD+0.285<br>KET+ONIT+ONITQ3                | 2.96E-14.*exp(1000./T) | 1 |
| R361d | OLNDQ+OLNDQ=NO2+NQ2+0.504<br>HCHO+1.21 ALD+0.285 KET+ONITQ                         | 2.96E-14.*exp(1000./T) | 1 |
| R361e | OLNDQ+OLNDQ2=NO2+NQ2+NQ2+0.5<br>04 HCHO+1.21 ALD+0.285<br>KET+ONITQ+ONITQ2         | 2.96E-14.*exp(1000./T) | 1 |
| R361f | OLNDQ+OLNDQ3=NO2+NQ2+NQ2+0.5<br>04 HCHO+1.21 ALD+0.285<br>KET+ONITQ+ONITQ3         | 2.96E-14.*exp(1000./T) | 1 |
| R361g | OLNDQ2+OLNDQ2=NQ2+NQ2+0.504<br>HCHO+1.21 ALD+0.285 KET+ONITQ2                      | 2.96E-14.*exp(1000./T) | 1 |
| R361h | OLNDQ2+OLNDQ3=NQ2+NQ2+0.504<br>HCHO+1.21 ALD+0.285<br>KET+ONITQ2+ONITQ3            | 2.96E-14.*exp(1000./T) | 1 |
| R361i | OLNDQ3+OLNDQ3=NQ2+0.504<br>HCHO+1.21 ALD+0.285 KET+ONITQ3                          | 2.96E-14.*exp(1000./T) | 1 |
| R362  | XO2+XO2=   | 7.13E-17.*exp(2950./T) | 1 |
| R363  | XO2+RCO3=ETHP +CO2   | 2.96E-14.*exp(1000./T) | 1 |

#### Oxygen Isotope Exchange

|              |                                      |                              |   |
|--------------|--------------------------------------|------------------------------|---|
| O_Exchange1  | Q3P+O2=O3P+O2                        | 2.9E-12.*0.21.*M             | 3 |
| O_Exchange2  | Q1D+O2=O1D+O2                        | 2.9E-12.*0.21.*M             | 3 |
| O_Exchange3  | Q1D+NO=O1D+NQ                        | 3.7E-11                      | 3 |
| O_Exchange4  | O1D+NQ=Q1D+NO                        | 3.7E-11                      | 3 |
| O_Exchange5  | Q3P+NO=O3P+NQ                        | 3.7E-11                      | 3 |
| O_Exchange6  | O3P+NQ=Q3P+NO                        | 3.7E-11                      | 3 |
| O_Exchange7  | QH+H2O=OH+H2O                        | 2.3E-13*exp(-<br>2100/T)*H2O | 3 |
| O_Exchange8  | QH+O2=OH+O2                          | 1.0E-17*0.21*M               | 3 |
| O_Exchange9  | QH+HO2=OH+HOQ                        | 1.E-11*exp(400/T)            | 3 |
| O_Exchange10 | OH+HOQ=0.5QH+0.5HO2+0.5OH+0.5H<br>OQ | 1.E-11*exp(400/T)            | 3 |

|              |  |                        |   |
|--------------|--|------------------------|---|
| O_Exchange11 | $QH + HOQ = 0.5OH + 0.5HQ2 + 0.5QH + 0.5HOQ$ | $1.E-11 * \exp(400/T)$ | 3 |
| O_Exchange12 | $OH + HQ2 = QH + HOQ$                        | $1.E-11 * \exp(400/T)$ | 3 |
| O_Exchange13 | $HOQ + O2 = HO2 + O2$                        | $3.0E-17 * 0.21 * M$   | 3 |
| O_Exchange14 | $HQ2 + O2 = HO2 + O2$                        | $3.0E-17 * 0.21 * M$   | 3 |
| O_Exchange15 | $NQ + NO2 = NO + NOQ$                        | $3.6E-14$              | 3 |
| O_Exchange16 | $NO + NOQ = 0.5NQ + 0.5NO2 + 0.5NO + 0.5HOQ$ | $3.6E-14$              | 3 |
| O_Exchange17 | $NQ + NOQ = 0.5NO + 0.5NQ2 + 0.5NQ + 0.5HOQ$ | $3.6E-14$              | 3 |
| O_Exchange18 | $NO + NQ2 = NQ + NOQ$                        | $3.6E-14$              | 3 |
| O_Exchange19 | $NOQ + O2 = NO2 + O2$                        | $1.E-24 * 0.21 * M$    | 3 |
| O_Exchange20 | $NQ2 + O2 = NO2 + O2$                        | $1.E-24 * 0.21 * M$    | 3 |
| O_Exchange21 | $QH + NO = OH + NQ$                          | $1.8E-11$              | 3 |
| O_Exchange22 | $OH + NQ = QH + NO$                          | $1.8E-11$              | 3 |
| O_Exchange23 | $QH + NO2 = OH + NOQ$                        | $1.0E-11$              | 3 |
| O_Exchange24 | $OH + NOQ = 0.5QH + 0.5NO2 + 0.5OH + 0.5HOQ$ | $1.0E-11$              | 3 |
| O_Exchange25 | $QH + NOQ = 0.5OH + 0.5NQ2 + 0.5QH + 0.5HOQ$ | $1.0E-11$              | 3 |
| O_Exchange26 | $OH + NQ2 = QH + NOQ$                        | $1.0E-11$              | 3 |

Note 1, (Goliff et al., 2013)

Note 2, (Atkinson et al., 2006)

Note 3, (Lyons, 2001)

**Table S4.** The RACM2 Chemical Mechanism: Troe Reaction Parameters.

| Reaction Rate Label | $k_0^{300} (\text{cm}^6 \text{s}^{-1})$ | n   | $k_\infty^{300} (\text{cm}^3 \text{s}^{-1})$ | m    | Note |
|---------------------|---|-----|--|------|------|
| K_O3P_NO            | 9.00E-32                                | 1.5 | 3.00E-11                                     | 0    | 1    |
| K_O3P_NO2           | 2.5E-31                                 | 1.8 | 2.2E-11                                      | 0.7  | 1    |
| K_OH_NO2_HONO2      | 1.8E-30                                 | 3.0 | 2.8E-11                                      | 0    | 1    |
| K_NO2_NO3           | 2.0E-30                                 | 4.4 | 1.4E-12                                      | 0.7  | 1    |
| K_HO2_NO2           | 2.0E-31                                 | 3.4 | 2.9E-12                                      | 1.1  | 1    |
| K_OH_SO2            | 3.3E-31                                 | 4.3 | 1.6E-12                                      | 0    | 1    |
| K_OH_ETE            | 1.0E-28                                 | 4.5 | 8.8E-12                                      | 0.85 | 1    |
| K_OH_ACE            | 5.5E-30                                 | 0   | 8.3E-13                                      | -2.0 | 1    |
| K_ACO3_NO2          | 9.7E-29                                 | 5.6 | 9.3E-12                                      | 1.5  | 1    |

Note 1, (Goliff et al., 2013)

**Table S5.** The RACM2 Chemical Mechanism: Troe Equilibrium Reactions

| Reaction Rate Label | A       | B      | $k_0^{300}(\text{cm}^6 \text{s}^{-1})$ | n   | $k_\infty^{300} (\text{cm}^3 \text{s}^{-1})$ | m   | Note |
|---------------------|---------|--------|--|-----|--|-----|------|
| K_N2O5              | 3.7E26  | 11,000 | 2.2E-30                                | 3.9 | 1.5E-12                                      | 0.7 | 1    |
| K_HO2NO2            | 4.76E26 | 10,900 | 2.00E-31                               | 3.4 | 2.9E-12                                      | 1.1 | 1    |
| K_PAN               | 1.16E28 | 13,954 | 9.70E-29                               | 5.6 | 9.30E-12                                     | 1.5 | 1    |

Note 1, (Goliff et al., 2013)

**Table S6.** The RACM2 Chemical Mechanism: Reactions with Special Rate Expressions.

| Reaction Rate Label | Rate Constant Expression  | Note |
|---------------------|---|------|
| K_HO2_NO_HNO3       | $k_1 = 3.45E-12 * \exp(270/T)$<br>$k_2 = (530/T) + (4.8E-6) * \text{pressure} - 1.73$<br>$k = k_1 * k_2 / 100$                                | 1    |
| K_OH_HNO3           | $k_0 = 2.4 E-14 * \exp(460/T)$<br>$k_2 = 2.4E-17 * \exp(2199/T)$<br>$k_3 = 6.5E-34 * \exp(1335/T) * [M]$<br>$k = k_0 + k_3 / (1 + k_3 / k_2)$ | 1    |
| K_OH_CO             | $1.44E-13 * (1 + 0.8 * [M]) / 4E19$   | 1    |

Note 1, (Goliff et al., 2013)

**Table S7.** Addition of heterogeneous reactions into ICOIN-RACM2 Mechanism (ICOIN-RACM2(het)).

| Reaction No. | Reaction   | $k_{\text{het}} (\text{s}^{-1})^{\text{a}}$ |
|--------------|--|---|
| Het_01       | $\text{NO}_2 = 0.5\text{HNO}_3 + 0.5\text{HONO}$   | 2.67E-6                                     |
| Het_01a      | $\text{NOQ} = 0.5\text{HNO}_2\text{Q} + 0.5\text{HONQ}$  | 2.67E-6                                     |
| Het_01b      | $\text{NQ}_2 = 0.5\text{HNOQ}_2 + 0.5\text{HQNQ}$  | 2.67E-6                                     |
| Het_02       | $\text{N}_2\text{O}_5 = \text{HNO}_3 + \text{HNO}_3$   | 4E-4  |
| Het_02a      | $\text{N}_2\text{O}_4\text{Q} = (2/5)\text{HNO}_2\text{Q} + (2/5)\text{HNO}_3 + (3/5)\text{HNO}_3 + (3/5)\text{HNO}_2\text{Q}$                                 | 4E-4  |
| Het_02b      | $\text{N}_2\text{O}_3\text{Q}_2 = 0.3\text{HNO}_3 + 0.6\text{HNO}_2\text{Q} + 0.1\text{HNOQ}_2 + 0.1\text{HNO}_3 + 0.6\text{HNO}_2\text{Q} + 0.3\text{HNOQ}_2$ | 4E-4  |
| Het_02c      | $\text{N}_2\text{O}_2\text{Q}_3 = 0.1\text{HNO}_3 + 0.6\text{HNO}_2\text{Q} + 0.3\text{HNOQ}_2 + 0.3\text{HNO}_2\text{Q} + 0.6\text{HNOQ}_2 + 0.1\text{HNQ}_3$ | 4E-4  |
| Het_02d      | $\text{N}_2\text{OQ}_4 = 0.4\text{HNO}_2\text{Q} + 0.6\text{HNOQ}_2 + 0.6\text{HNOQ}_2 + 0.4\text{HNQ}_3$  | 4E-4  |
| Het_02e      | $\text{N}_2\text{Q}_5 = \text{HNQ}_3 + \text{HNOQ}_2$  | 4E-4  |

<sup>a</sup>The calculation of the pseudo-first order heterogeneous reaction rates was discussed in the manuscript for demonstration-purposes of diel cycles of  $\Delta^{17}\text{O}$  only. These reaction rates should not be generalized for all model simulations.

## References

- Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and IUPAC Subcommittee: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - gas phase reactions of organic species, *Atmospheric Chemistry and Physics*, 6, 3625–4055, <https://doi.org/10.5194/acp-6-3625-2006>, 2006.
- Goliff, W. S., Stockwell, W. R., and Lawson, C. V.: The regional atmospheric chemistry mechanism, version 2, *Atmospheric Environment*, 68, 174–185, <https://doi.org/10.1016/j.atmosenv.2012.11.038>, 2013.
- Lyons, J. R.: Transfer of mass-independent fractionation in ozone to other oxygen-containing radicals in the atmosphere, *Geophysical Research Letters*, 28, 3231–3234, 2001.
- Wolfe, G. M., Marvin, M. R., Roberts, S. J., Travis, K. R., and Liao, J.: The Framework for 0-D Atmospheric Modeling (F0AM) v3.1, *Geoscientific Model Development*, 9, 3309–3319, <https://doi.org/10.5194/gmd-9-3309-2016>, 2016.