# The Chemical Mechanism of MECCA

KPP version: `2.2.3_rs3`

MECCA version: `4.5.0gmdd`

Date: October 5, 2020

Batch file: `latex`

Integrator: `rosenbrock_posdef`

Gas equation file: `gas.eqn`

Replacement file:

Selected reactions:
"`!Ara`"

Number of aerosol phases: 1

Number of species in selected mechanism:

| | |
|---|---|
| Gas phase: | 708 |
| Aqueous phase: | 482 |
| All species: | 1190 |

Number of reactions in selected mechanism:

| | |
|---|---|
| Gas phase (Gnnn): | 1815 |
| Aqueous phase (Annn): | 402 |
| Henry (Hnnn): | 735 |
| Photolysis (Jnnn): | 385 |
| Aqueous phase photolysis (PHnnn): | 27 |
| Heterogeneous (HETnnn): | 21 |
| Equilibria (EQnn): | 136 |
| Isotope exchange (IEXnnn): | 0 |
| Tagging equations (TAGnnn): | 0 |
| Dummy (Dnn): | 1 |
| All equations: | 3522 |

Table 1: Gas phase reactions

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G1000 | UpStTrG | $O_2 + O(^1D) \rightarrow O(^3P) + O_2$ | 3.3E-11*EXP(55./temp) | Burkholder et al. (2015) |
| G1001 | UpStTrG | $O_2 + O(^3P) \rightarrow O_3$ | 6.0E-34*((temp/300.)**(-2.4)) *cair | Burkholder et al. (2015) |
| G1002a | UpStG | $O_3 + O(^1D) \rightarrow 2\ O_2$ | 1.2E-10 | Burkholder et al. (2015)* |
| G1002b | UpG | $O_3 + O(^1D) \rightarrow O_2 + 2\ O(^3P)$ | 1.2E-10 | Burkholder et al. (2015) |
| G1003 | UpStG | $O_3 + O(^3P) \rightarrow 2\ O_2$ | 8.0E-12*EXP(-2060./temp) | Burkholder et al. (2015) |
| G1004 | UpG | $O_2 + O^+ \rightarrow O_2^+ + O(^3P)$ | k_Op_O2(temp,temp_ion) | Fuller-Rowell (1993) |
| G1101 | UpG | $O_2^+ + e^- \rightarrow 2\ O(^3P)$ | 2.7E-7*(300./temp_elec)**(.7) | Fuller-Rowell (1993) |
| G2100 | UpStTrG | $H + O_2 \rightarrow HO_2$ | k_3rd(temp,cair,4.4E-32,1.3, 7.5E-11,-0.2,0.6) | Burkholder et al. (2015) |
| G2101 | UpStG | $H + O_3 \rightarrow OH + O_2$ | 1.4E-10*EXP(-470./temp) | Burkholder et al. (2015) |
| G2102 | UpStG | $H_2 + O(^1D) \rightarrow H + OH$ | 1.2E-10 | Burkholder et al. (2015) |
| G2103 | UpStG | $OH + O(^3P) \rightarrow H + O_2$ | 1.8E-11*EXP(180./temp) | Burkholder et al. (2015) |
| G2104 | UpStTrG | $OH + O_3 \rightarrow HO_2 + O_2$ | 1.7E-12*EXP(-940./temp) | Burkholder et al. (2015) |
| G2105 | UpStTrG | $OH + H_2 \rightarrow H_2O + H$ | 2.8E-12*EXP(-1800./temp) | Burkholder et al. (2015) |
| G2106 | UpStG | $HO_2 + O(^3P) \rightarrow OH + O_2$ | 3.E-11*EXP(200./temp) | Burkholder et al. (2015) |
| G2107 | UpStTrG | $HO_2 + O_3 \rightarrow OH + 2\ O_2$ | 1.E-14*EXP(-490./temp) | Burkholder et al. (2015) |
| G2108a | UpStG | $HO_2 + H \rightarrow 2\ OH$ | 7.2E-11 | Burkholder et al. (2015) |
| G2108b | UpStG | $HO_2 + H \rightarrow H_2 + O_2$ | 6.9E-12 | Burkholder et al. (2015) |
| G2108c | UpStG | $HO_2 + H \rightarrow O(^3P) + H_2O$ | 1.6E-12 | Burkholder et al. (2015) |
| G2109 | UpStTrG | $HO_2 + OH \rightarrow H_2O + O_2$ | 4.8E-11*EXP(250./temp) | Burkholder et al. (2015) |
| G2110 | UpStTrG | $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$ | k_HO2_HO2 | Burkholder et al. (2015)* |
| G2111 | UpStTrG | $H_2O + O(^1D) \rightarrow 2\ OH$ | 1.63E-10*EXP(60./temp) | Burkholder et al. (2015) |
| G2112 | UpStTrG | $H_2O_2 + OH \rightarrow H_2O + HO_2$ | 1.8E-12 | Burkholder et al. (2015) |
| G2113 | UpG | $H_2 + O(^3P) \rightarrow H + OH$ | 1.60E-11*EXP(-4570./temp) | Roble (1995) |
| G2114a | UpG | $OH + OH \rightarrow H_2O + O(^3P)$ | 4.20E-12*EXP(-240./temp) | Sander et al. (2003) |
| G2114b | UpG | $OH + OH \rightarrow H_2O_2$ | k_3rd(temp,cair,6.9E-31,1.0, 2.6E-11,0.,0.6) | Burkholder et al. (2015) |
| G2115 | UpG | $H + H \rightarrow H_2$ | 5.7E-32*(300./temp)**(1.6)*cair | Roble (1995) |
| G2116 | UpG | $H_2O_2 + O(^3P) \rightarrow OH + HO_2$ | 1.40E-12*EXP(-2000./temp) | Sander et al. (2003) |
| G2117 | UpStTrG | $H_2O + H_2O \rightarrow (H_2O)_2$ | 6.521E-26*temp*EXP(1851.09/temp) *EXP(-5.10485E-3*temp) | Scribano et al. (2006)* |
| G2118 | UpStTrG | $(H_2O)_2 \rightarrow H_2O + H_2O$ | 1.E0 | see note* |
| G3001 | UpGN | $NO^+ + e^- \rightarrow .15\ N + .85\ N(^2D) + O(^3P)$ | 4.2E-7*(300./temp_elec)**(0.85) | Bailey et al. (2002) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G3002 | UpGN | $N_2^+ + e^- \rightarrow .88\ N + 1.12\ N(^2D)$ | 1.8E-7*(temp_elec/300.)**(-0.39) | Swaminathan et al. (1998) |
| G3003 | UpGN | $N(^2D) + e^- \rightarrow N + e^-$ | 3.8E-12*(temp_elec)**(.81) | Swaminathan et al. (1998) |
| G3100 | UpStGN | $N + O_2 \rightarrow NO + O(^3P)$ | 1.5E-11*EXP(-3600./temp) | Burkholder et al. (2015) |
| G3101 | UpStTrGN | $N_2 + O(^1D) \rightarrow O(^3P) + N_2$ | 2.15E-11*EXP(110./temp) | Burkholder et al. (2015) |
| G3102a | UpStGN | $N_2O + O(^1D) \rightarrow 2\ NO$ | 7.259E-11*EXP(20./temp) | Burkholder et al. (2015) |
| G3102b | StGN | $N_2O + O(^1D) \rightarrow N_2 + O_2$ | 4.641E-11*EXP(20./temp) | Burkholder et al. (2015) |
| G3103 | UpStTrGN | $NO + O_3 \rightarrow NO_2 + O_2$ | 3.0E-12*EXP(-1500./temp) | Burkholder et al. (2015) |
| G3104 | UpStGN | $NO + N \rightarrow O(^3P) + N_2$ | 2.1E-11*EXP(100./temp) | Burkholder et al. (2015) |
| G3105 | UpStGN | $NO_2 + O(^3P) \rightarrow NO + O_2$ | 5.1E-12*EXP(210./temp) | Burkholder et al. (2015) |
| G3106 | StTrGN | $NO_2 + O_3 \rightarrow NO_3 + O_2$ | 1.2E-13*EXP(-2450./temp) | Burkholder et al. (2015) |
| G3107 | UpStGN | $NO_2 + N \rightarrow N_2O + O(^3P)$ | 5.8E-12*EXP(220./temp) | Burkholder et al. (2015) |
| G3108 | StTrGN | $NO_3 + NO \rightarrow 2\ NO_2$ | 1.5E-11*EXP(170./temp) | Burkholder et al. (2015) |
| G3109 | UpStTrGN | $NO_3 + NO_2 \rightarrow N_2O_5$ | k_NO3_NO2 | Burkholder et al. (2015)* |
| G3110 | StTrGN | $N_2O_5 \rightarrow NO_2 + NO_3$ | k_NO3_NO2/(5.8E-27*EXP(10840./ temp)) | Burkholder et al. (2015)* |
| G3111 | UpGN | $N(^2D) + NO \rightarrow N_2 + O(^3P)$ | 6.70E-11 | Fuller-Rowell (1993) |
| G3112 | UpGN | $N(^2D) + O_2 \rightarrow NO + O(^3P)$ | 6.20E-12*(temp/300.) | Duff et al. (2003) |
| G3113 | UpGN | $N(^2D) + O(^3P) \rightarrow N + O(^3P)$ | 6.90E-13 | Fell et al. (1990) |
| G3114 | UpGN | $N(^2D) + O_3 \rightarrow NO + O_2$ | 0.80E-16 | Sander et al. (2003) |
| G3115 | UpGN | $NO + O(^3P) \rightarrow NO_2$ | k_3rd(temp,cair,9.0E-32,1.5, 3.0E-11,0.0,0.6) | Burkholder et al. (2015) |
| G3116 | UpGN | $NO_2 + O(^3P) \rightarrow NO_3$ | k_3rd(temp,cair,2.5E-31,1.8, 2.2E-11,0.7,0.6) | Burkholder et al. (2015) |
| G3117 | UpGN | $N(^2D) \rightarrow N$ | 10.6 | Fuller-Rowell (1993) |
| G3118 | UpGN | $N^+ + O_2 \rightarrow NO + O^+$ | 3.66E-11 | Barth (1992) |
| G3119 | UpGN | $N_2^+ + O(^3P) \rightarrow NO^+ + N(^2D)$ | k_N2_O(temp,temp_ion) | Fuller-Rowell (1993) |
| G3120a | UpGN | $N^+ + O_2 \rightarrow NO^+ + O(^3P)$ | 2.60E-10 | Fuller-Rowell (1993) |
| G3120b | UpGN | $N^+ + O_2 \rightarrow O_2^+ + N$ | 3.10E-10 | Swaminathan et al. (1998) |
| G3121 | UpGN | $N^+ + O(^3P) \rightarrow O^+ + N$ | 1.00E-12 | Fuller-Rowell (1993) |
| G3122 | UpGN | $O_2^+ + N \rightarrow NO^+ + O(^3P)$ | 1.20E-10 | Fuller-Rowell (1993) |
| G3123 | UpGN | $O_2^+ + NO \rightarrow NO^+ + O_2$ | 4.40E-10 | Fuller-Rowell (1993) |
| G3124 | UpGN | $O^+ + N_2 \rightarrow NO^+ + N$ | k_Op_N2(temp,temp_ion) | Fuller-Rowell (1993) |
| G3125 | UpGN | $N_2^+ + O_2 \rightarrow N_2 + O_2^+$ | 5.10E-11*(temp/300.)**(-0.8) | Fuller-Rowell (1993) |
| G3200 | TrGN | $NO + OH \rightarrow HONO$ | k_3rd(temp,cair,7.0E-31,2.6, 3.6E-11,0.1,0.6) | Burkholder et al. (2015) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G3201 | UpStTrGN | $NO + HO_2 \rightarrow NO_2 + OH$ | 3.3E-12*EXP(270./temp) | Burkholder et al. (2015) |
| G3202a | UpStTrGN | $NO_2 + OH \rightarrow HNO_3$ | (1.-alpha_HOONO) * k_NO2_OH | Amedro et al. (2020) |
| G3202b | UpStTrGN | $NO_2 + OH \rightarrow HOONO$ | alpha_HOONO * k_NO2_OH | Amedro et al. (2020) |
| G3203 | StTrGN | $NO_2 + HO_2 \rightarrow HNO_4$ | k_NO2_HO2 | Burkholder et al. (2015)* |
| G3204 | TrGN | $NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$ | 3.5E-12 | Burkholder et al. (2015) |
| G3205 | TrGN | $HONO + OH \rightarrow NO_2 + H_2O$ | 1.8E-11*EXP(-390./temp) | Burkholder et al. (2015) |
| G3206 | StTrGN | $HNO_3 + OH \rightarrow H_2O + NO_3$ | k_HNO3_OH | Dulitz et al. (2018)* |
| G3207 | StTrGN | $HNO_4 \rightarrow NO_2 + HO_2$ | k_NO2_HO2/(2.1E-27*EXP(10900./ temp)) | Burkholder et al. (2015)* |
| G3208 | StTrGN | $HNO_4 + OH \rightarrow NO_2 + H_2O$ | 1.3E-12*EXP(380./temp) | Burkholder et al. (2015) |
| G3209 | TrGN | $NH_3 + OH \rightarrow NH_2 + H_2O$ | 1.7E-12*EXP(-710./temp) | Kohlmann and Poppe (1999) |
| G3210 | TrGN | $NH_2 + O_3 \rightarrow NH_2O + O_2$ | 4.3E-12*EXP(-930./temp) | Kohlmann and Poppe (1999) |
| G3211 | TrGN | $NH_2 + HO_2 \rightarrow NH_2O + OH$ | 4.8E-07*EXP(-628./temp)*(temp) **(-1.32) | Kohlmann and Poppe (1999) |
| G3212 | TrGN | $NH_2 + HO_2 \rightarrow HNO + H_2O$ | 9.4E-09*EXP(-356./temp)*(temp) **(-1.12) | Kohlmann and Poppe (1999) |
| G3213 | TrGN | $NH_2 + NO \rightarrow HO_2 + OH + N_2$ | 1.92E-12*((temp/298.)**(-1.5)) | Kohlmann and Poppe (1999) |
| G3214 | TrGN | $NH_2 + NO \rightarrow N_2 + H_2O$ | 1.41E-11*((temp/298.)**(-1.5)) | Kohlmann and Poppe (1999) |
| G3215 | TrGN | $NH_2 + NO_2 \rightarrow N_2O + H_2O$ | 1.2E-11*((temp/298.)**(-2.0)) | Kohlmann and Poppe (1999) |
| G3216 | TrGN | $NH_2 + NO_2 \rightarrow NH_2O + NO$ | 0.8E-11*((temp/298.)**(-2.0)) | Kohlmann and Poppe (1999) |
| G3217 | TrGN | $NH_2O + O_3 \rightarrow NH_2 + O_2$ | 1.2E-14 | Kohlmann and Poppe (1999) |
| G3218 | TrGN | $NH_2O \rightarrow NHOH$ | 1.3E3 | Kohlmann and Poppe (1999) |
| G3219 | TrGN | $HNO + OH \rightarrow NO + H_2O$ | 8.0E-11*EXP(-500./temp) | Kohlmann and Poppe (1999) |
| G3220 | TrGN | $HNO + NHOH \rightarrow NH_2OH + NO$ | 1.66E-12*EXP(-1500./temp) | Kohlmann and Poppe (1999) |
| G3221 | TrGN | $HNO + NO_2 \rightarrow HONO + NO$ | 1.0E-12*EXP(-1000./temp) | Kohlmann and Poppe (1999) |
| G3222 | TrGN | $NHOH + OH \rightarrow HNO + H_2O$ | 1.66E-12 | Kohlmann and Poppe (1999) |
| G3223 | TrGN | $NH_2OH + OH \rightarrow NHOH + H_2O$ | 4.13E-11*EXP(-2138./temp) | Kohlmann and Poppe (1999) |
| G3224 | TrGN | $HNO + O_2 \rightarrow HO_2 + NO$ | 3.65E-14*EXP(-4600./temp) | Kohlmann and Poppe (1999) |
| G3225 | UpGN | $N + OH \rightarrow NO + H$ | 5.00E-11 | Roble (1995) |
| G3226 | UpGN | $NO_2 + H \rightarrow NO + OH$ | 4.00E-10*EXP(-340./temp) | Sander et al. (2003) |
| G3227 | UpStTrGN | $HOONO \rightarrow NO_2 + OH$ | (alpha_HOONO*k_NO2_OH) /(3.5E-27*EXP(10135./temp)) | see note* |
| G3228 | UpStTrGN | $HOONO + OH \rightarrow H_2O + NO_3$ | 1.3E-12*EXP(380./temp) | Burkholder et al. (2015)* |
| G4100 | UpStG | $CH_4 + O(^1D) \rightarrow .75\ CH_3 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$ | 1.75E-10 | Burkholder et al. (2015) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G4101 | StTrG | $CH_4 + OH \rightarrow CH_3 + H_2O$ | `1.85E-20*EXP(2.82*LOG(temp) -987./temp)` | Atkinson (2003) |
| G4102 | TrG | $CH_3OH + OH \rightarrow .85\ HCHO + .85\ HO_2 + .15\ CH_3O + H_2O$ | `6.38E-18*((temp)**2)*EXP(144./temp)` | Atkinson et al. (2006) |
| G4103a | StTrG | $CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$ | `3.8E-13*EXP(780./temp)/(1.+1./498.*EXP(1160./temp))` | Atkinson et al. (2006) |
| G4103b | StTrG | $CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$ | `3.8E-13*EXP(780./temp)/(1.+498.*EXP(-1160./temp))` | Atkinson et al. (2006) |
| G4104a | StTrGN | $CH_3O_2 + NO \rightarrow CH_3O + NO_2$ | `2.3E-12*EXP(360./temp)*(1.-beta_CH3NO3)` | Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998) |
| G4104b | StTrGN | $CH_3O_2 + NO \rightarrow CH_3ONO_2$ | `2.3E-12*EXP(360./temp)*beta_CH3NO3` | Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)* |
| G4105 | TrGN | $CH_3O_2 + NO_3 \rightarrow CH_3O + NO_2 + O_2$ | `1.2E-12` | Atkinson et al. (2006) |
| G4106a | StTrG | $CH_3O_2 \rightarrow CH_3O + .5\ O_2$ | `7.4E-13*EXP(-520./temp)*RO2*2.` | Atkinson et al. (2006) |
| G4106b | StTrG | $CH_3O_2 \rightarrow .5\ HCHO + .5\ CH_3OH + .5\ O_2$ | `(k_CH3O2-7.4E-13*EXP(-520./temp))*RO2*2.` | Atkinson et al. (2006) |
| G4107 | StTrG | $CH_3OOH + OH \rightarrow .6\ CH_3O_2 + .4\ HCHO + .4\ OH + H_2O$ | `k_CH3OOH_OH` | Wallington et al. (2018) |
| G4108 | StTrG | $HCHO + OH \rightarrow CO + H_2O + HO_2$ | `9.52E-18*EXP(2.03*LOG(temp) +636./temp)` | Sivakumaran et al. (2003) |
| G4109 | TrGN | $HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$ | `3.4E-13*EXP(-1900./temp)` | Burkholder et al. (2015)* |
| G4110 | UpStTrG | $CO + OH \rightarrow H + CO_2$ | `(1.57E-13+cair*3.54E-33)` | McCabe et al. (2001) |
| G4111 | TrG | $HCOOH + OH \rightarrow CO_2 + HO_2 + H_2O$ | `2.94E-14*exp(786./temp) +9.85E-13*EXP(-1036./temp)` | Paulot et al. (2011) |
| G4112 | UpStG | $CO + O(^3P) \rightarrow CO_2$ | `6.60E-33*EXP(-1103./temp)` | Roble (1995) |
| G4113 | UpStG | $CH_4 + O(^3P) \rightarrow .51\ CH_3 + .51\ OH + .49\ CH_3O + .49\ H$ | `6.03E-18*(temp)**(2.17) *EXP(-3619./temp)` | Roble (1995), Garton et al. (2003), Espinosa-Garcia and Garcia-Bernáldez (2000) |
| G4114 | StTrGN | $CH_3O_2 + NO_2 \rightarrow CH_3O_2NO_2$ | `k_NO2_CH3O2` | Burkholder et al. (2015) |
| G4115 | StTrGN | $CH_3O_2NO_2 \rightarrow CH_3O_2 + NO_2$ | `k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))` | Burkholder et al. (2015)* |
| G4116 | StTrGN | $CH_3O_2NO_2 + OH \rightarrow HCHO + NO_3 + H_2O$ | `3.00E-14` | see note* |
| G4117 | StTrGN | $CH_3ONO_2 + OH \rightarrow H_2O + HCHO + NO_2$ | `4.0E-13*EXP(-845./temp)` | Atkinson et al. (2006) |
| G4118 | StTrG | $CH_3O \rightarrow HO_2 + HCHO$ | `1.3E-14*exp(-663./temp)*c(ind_O2)` | Chai et al. (2014) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G4119a | StTrGN | $CH_3O + NO_2 \rightarrow CH_3ONO_2$ | k_3rd_iupac(temp,cair,8.1E-29, 4.5,2.1E-11,0.,0.44) | Atkinson et al. (2006) |
| G4119b | StTrGN | $CH_3O + NO_2 \rightarrow HCHO + HONO$ | 9.6E-12*EXP(-1150./temp) | Atkinson et al. (2006) |
| G4120a | StTrGN | $CH_3O + NO \rightarrow CH_3ONO$ | k_3rd_iupac(temp,cair,2.6E-29, 2.8,3.3E-11,0.6,REAL(EXP(-temp/ 900.),SP)) | Atkinson et al. (2006) |
| G4120b | StTrGN | $CH_3O + NO \rightarrow HCHO + HNO$ | 2.3E-12*(temp/300.)**(0.7) | Atkinson et al. (2006) |
| G4121 | StTrG | $CH_3O_2 + O_3 \rightarrow CH_3O + 2\ O_2$ | 2.9E-16*exp(-1000./temp) | Burkholder et al. (2015) |
| G4122 | StTrGN | $CH_3ONO + OH \rightarrow H_2O + HCHO + NO$ | 1.E-10*exp(-1764./temp) | Nielsen et al. (1991) |
| G4123 | StTrG | $HCHO + HO_2 \rightarrow HOCH_2O_2$ | 9.7E-15*EXP(625./temp) | Atkinson et al. (2006) |
| G4124 | StTrG | $HOCH_2O_2 \rightarrow HCHO + HO_2$ | 2.4E12*EXP(-7000./temp) | Atkinson et al. (2006) |
| G4125 | StTrG | $HOCH_2O_2 + HO_2 \rightarrow .5\ HOCH_2OOH + .5\ HCOOH + .2\ OH + .2\ HO_2 + .3\ H_2O + .8\ O_2$ | 5.6E-15*EXP(2300./temp) | Atkinson et al. (2006) |
| G4126 | StTrGN | $HOCH_2O_2 + NO \rightarrow NO_2 + HO_2 + HCOOH$ | 0.7275*2.3E-12*EXP(360./temp) | Atkinson et al. (2006)* |
| G4127 | StTrGN | $HOCH_2O_2 + NO_3 \rightarrow NO_2 + HO_2 + HCOOH$ | 1.2E-12 | see note* |
| G4129a | StTrG | $HOCH_2O_2 \rightarrow HCOOH + HO_2$ | (k_CH3O2*5.5E-12)**(0.5)*RO2*2. | Atkinson et al. (2006) |
| G4129b | StTrG | $HOCH_2O_2 \rightarrow .5\ HCOOH + .5\ HOCH_2OH + .5\ O_2$ | (k_CH3O2*5.7E-14*EXP(750./temp)) **(0.5)*RO2*2. | Atkinson et al. (2006) |
| G4130a | StTrG | $HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$ | k_ROOHRO | Taraborrelli (2010)* |
| G4130b | StTrG | $HOCH_2OOH + OH \rightarrow HCOOH + H_2O + OH$ | k_ROHRO + k_s*f_sOOH*f_sOH | Taraborrelli (2010)* |
| G4132 | StTrG | $HOCH_2OH + OH \rightarrow HO_2 + HCOOH + H_2O$ | 2.*k_ROHRO + k_s*f_sOH*f_sOH | Taraborrelli (2010)* |
| G4133 | StTrG | $CH_3O_2 + OH \rightarrow CH_3O + HO_2$ | 1.4E-10 | Bossolasco et al. (2014)* |
| G4134 | StTrG | $CH_2OO \rightarrow CO + HO_2 + OH$ | 1.124E+14*EXP(-10000./temp) | see note* |
| G4135 | StTrG | $CH_2OO + H_2O \rightarrow HOCH_2OOH$ | k_CH2OO_NO2*3.6E-6 | Ouyang et al. (2013)* |
| G4136 | StTrG | $CH_2OO + (H_2O)_2 \rightarrow HOCH_2OOH + H_2O$ | 5.2E-12 | Chao et al. (2015), Lewis et al. (2015)* |
| G4137 | StTrGN | $CH_2OO + NO \rightarrow HCHO + NO_2$ | 6.E-14 | Welz et al. (2012)* |
| G4138 | StTrGN | $CH_2OO + NO_2 \rightarrow HCHO + NO_3$ | k_CH2OO_NO2 | Welz et al. (2012), Stone et al. (2014)* |
| G4140 | StTrG | $CH_2OO + CO \rightarrow HCHO + CO_2$ | 3.6E-14 | Vereecken et al. (2012) |
| G4141 | StTrG | $CH_2OO + HCOOH \rightarrow 2\ HCOOH$ | 1.E-10 | Welz et al. (2014)* |
| G4142 | StTrG | $CH_2OO + HCHO \rightarrow 2\ LCARBON$ | 1.7E-12 | Stone et al. (2014)* |
| G4143 | StTrG | $CH_2OO + CH_3OH \rightarrow 2\ LCARBON$ | 5.E-12 | Vereecken et al. (2012)* |
| G4144 | StTrG | $CH_2OO + CH_3O_2 \rightarrow 2\ LCARBON$ | 5.E-12 | Vereecken et al. (2012)* |
| G4145 | StTrG | $CH_2OO + HO_2 \rightarrow LCARBON$ | 5.E-12 | Vereecken et al. (2012) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G4146 | StTrG | $CH_2OO + O_3 \rightarrow HCHO + 2\ O_2$ | `1.E-12` | Vereecken et al. (2014) |
| G4147 | StTrG | $CH_2OO + CH_2OO \rightarrow 2\ HCHO + O_2$ | `6.E-11` | Buras et al. (2014) |
| G4148 | StTrGN | $HOCH_2O_2 + NO_2 \rightarrow HOCH_2O_2NO_2$ | `k_NO2_CH3O2` | see note* |
| G4149 | StTrGN | $HOCH_2O_2NO_2 \rightarrow HOCH_2O_2 + NO_2$ | `k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))` | Barnes et al. (1985)* |
| G4150 | StTrGN | $HOCH_2O_2NO_2 + OH \rightarrow HCOOH + NO_3 + H_2O$ | `9.50E-13*EXP(-650./temp)*f_sOH` | see note* |
| G4151 | StTrG | $CH_3 + O_2 \rightarrow CH_3O_2$ | `k_3rd_iupac(temp,cair,7.0E-31,3.,1.8E-12,-1.1,0.33)` | Atkinson et al. (2006) |
| G4152 | StTrG | $CH_3 + O_3 \rightarrow .956\ HCHO + .956\ H + .044\ CH_3O + O_2$ | `5.1E-12*exp(-210./temp)` | Albaladejo et al. (2002), Ogryzlo et al. (1981) |
| G4153 | StTrG | $CH_3 + O(^3P) \rightarrow .83\ HCHO + .83\ H + .17\ CO + .17\ H_2 + .17\ H$ | `1.3E-10` | Atkinson et al. (2006) |
| G4154 | StTrG | $CH_3O + O_3 \rightarrow CH_3O_2 + O_2$ | `2.53E-14` | Albaladejo et al. (2002)* |
| G4155 | StTrG | $CH_3O + O(^3P) \rightarrow .75\ CH_3 + .75\ O_2 + .25\ HCHO + .25\ OH$ | `2.5E-11` | Baulch et al. (2005) |
| G4156 | StTrG | $CH_3O_2 + O(^3P) \rightarrow CH_3O + O_2$ | `4.3E-11` | Zellner et al. (1988) |
| G4157 | StTrG | $HCHO + O(^3P) \rightarrow .7\ OH + .7\ CO + .3\ H + .3\ CO_2 + HO_2$ | `3.4E-11*EXP(-1600./temp)` | Burkholder et al. (2015) |
| G4158 | TrG | $CH_2OO^* \rightarrow .37\ CH_2OO + .47\ CO + .47\ H_2O + .16\ HO_2 + .16\ CO + .16\ OH$ | `KDEC` | Atkinson et al. (2006) |
| G4159 | TrGN | $HCN + OH \rightarrow H_2O + CN$ | `k_3rd(temp,cair,4.28E-33,1.0,REAL(4.25E-13*EXP(-1150./temp),SP),1.0,0.8)` | Kleinböhl et al. (2006) |
| G4160a | TrGN | $HCN + O(^1D) \rightarrow O(^3P) + HCN$ | `1.08E-10*EXP(105./temp)*0.15*EXP(200./temp)` | Strekowski et al. (2010) |
| G4160b | TrGN | $HCN + O(^1D) \rightarrow H + NCO$ | `1.08E-10*EXP(105./temp)*0.68/2.` | Strekowski et al. (2010)* |
| G4160c | TrGN | $HCN + O(^1D) \rightarrow OH + CN$ | `1.08E-10*EXP(105./temp)*(1.-(0.68/2.+0.15*EXP(200./temp)))` | Strekowski et al. (2010)* |
| G4161 | TrGN | $HCN + O(^3P) \rightarrow H + NCO$ | `1.0E-11*EXP(-4000./temp)` | Burkholder et al. (2015)* |
| G4162 | TrGN | $CN + O_2 \rightarrow NCO + O(^3P)$ | `1.2E-11*EXP(210./temp)*0.75` | Baulch et al. (2005) |
| G4163 | TrGN | $CN + O_2 \rightarrow CO + NO$ | `1.2E-11*EXP(210./temp)*0.25` | Baulch et al. (2005) |
| G4164 | TrGN | $NCO + O_2 \rightarrow CO_2 + NO$ | `7.E-15` | Becker et al. (2000)* |
| G42000 | TrGC | $C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$ | `1.49E-17*temp*temp*EXP(-499./temp)` | Atkinson et al. (2006) |
| G42001 | TrGC | $C_2H_4 + O_3 \rightarrow HCHO + CH_2OO^*$ | `9.1E-15*EXP(-2580./temp)` | Atkinson et al. (2006)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42002 | TrGC | $C_2H_4 + OH \rightarrow HOCH_2CH_2O_2$ | k_3rd_iupac(temp,cair,8.6E-29, 3.1,9.E-12,0.85,0.48) | Atkinson et al. (2006), Rickard and Pascoe (2009) |
| G42003 | TrGC | $C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$ | 7.5E-13*EXP(700./temp) | Burkholder et al. (2015) |
| G42004a | TrGCN | $C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$ | 2.55E-12*EXP(380./temp)*(1.-beta_ C2H5NO3) | Atkinson et al. (2006), Butkovskaya et al. (2010) |
| G42004b | TrGCN | $C_2H_5O_2 + NO \rightarrow C_2H_5ONO_2$ | 2.55E-12*EXP(380./temp)*beta_ C2H5NO3 | Atkinson et al. (2006), Butkovskaya et al. (2010) |
| G42005 | TrGCN | $C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$ | 2.3E-12 | Wallington et al. (2018) |
| G42006 | TrGC | $C_2H_5O_2 \rightarrow .8\ CH_3CHO + .6\ HO_2 + .2\ C_2H_5OH$ | 2.*(7.6E-14*k_CH3O2)**(.5)*RO2 | Sander et al. (2019), Atkinson et al. (2006) |
| G42007a | TrGC | $C_2H_5OOH + OH \rightarrow C_2H_5O_2 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G42007b | TrGC | $C_2H_5OOH + OH \rightarrow CH_3CHO + OH$ | k_s*f_sOOH | Sander et al. (2019) |
| G42008a | TrGC | $CH_3CHO + OH \rightarrow CH_3C(O) + H_2O$ | 4.4E-12*EXP(365./temp)*0.95 | Atkinson et al. (2006) |
| G42008b | TrGC | $CH_3CHO + OH \rightarrow HCOCH_2O_2 + H_2O$ | 4.4E-12*EXP(365./temp)*0.05 | Atkinson et al. (2006) |
| G42009 | TrGCN | $CH_3CHO + NO_3 \rightarrow CH_3C(O) + HNO_3$ | KNO3AL | Rickard and Pascoe (2009) |
| G42010 | TrGC | $CH_3COOH + OH \rightarrow CH_3 + CO_2 + H_2O$ | k_CH3CO2H_OH | Atkinson et al. (2006)* |
| G42011a | TrGC | $CH_3C(O)OO + HO_2 \rightarrow OH + CH_3 + CO_2$ | 5.20E-13*EXP(980./temp)*1.507*0.61 | Groß et al. (2014) |
| G42011b | TrGC | $CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$ | 5.20E-13*EXP(980./temp)*1.507*0.23 | Groß et al. (2014) |
| G42011c | TrGC | $CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$ | 5.20E-13*EXP(980./temp)*1.507*0.16 | Groß et al. (2014) |
| G42012 | TrGCN | $CH_3C(O)OO + NO \rightarrow CH_3 + CO_2 + NO_2$ | 8.1E-12*EXP(270./temp) | Tyndall et al. (2001a) |
| G42013 | TrGCN | $CH_3C(O)OO + NO_2 \rightarrow PAN$ | k_CH3CO3_NO2 | Burkholder et al. (2015)* |
| G42014 | TrGCN | $CH_3C(O)OO + NO_3 \rightarrow CH_3 + NO_2 + CO_2$ | 4.E-12 | Canosa-Mas et al. (1996) |
| G42017a | TrGC | $CH_3C(O)OO \rightarrow CH_3 + CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G42017b | TrGC | $CH_3C(O)OO \rightarrow CH_3COOH$ | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G42018 | TrGC | $CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$ | k_ROOHRO | Rickard and Pascoe (2009)* |
| G42020 | TrGCN | $PAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$ | 3.00E-14 | Rickard and Pascoe (2009) |
| G42021 | TrGCN | $PAN \rightarrow CH_3C(O)OO + NO_2$ | k_PAN_M | Burkholder et al. (2015)* |
| G42022a | TrGC | $C_2H_2 + OH \rightarrow GLYOX + OH$ | k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,-2.,0.6)*0.71 | Burkholder et al. (2015)* |
| G42022b | TrGC | $C_2H_2 + OH \rightarrow HCOOH + CO + HO_2$ | k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,-2.,0.6)*0.29 | Burkholder et al. (2015)* |
| G42023a | TrGC | $HOCH_2CHO + OH \rightarrow HOCH2CO + H_2O$ | 8.00E-12*0.80 | Atkinson et al. (2006) |
| G42023b | TrGC | $HOCH_2CHO + OH \rightarrow HOCHCHO + H_2O$ | 8.00E-12*0.20 | Atkinson et al. (2006) |
| G42024a | TrGC | $HOCH2CO + O_2 \rightarrow HOCH_2CO_3$ | 5.1E-12*(1.-1./(1+1.85E-18*cair)) | Atkinson et al. (2006), Beyersdorf et al. (2010)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42024b | TrGC | HOCH2CO + $O_2$ → OH + HCHO + $CO_2$ | `5.1E-12*1./(1+1.85E-18*cair)` | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42025 | TrGC | HOCHCHO → GLYOX + $HO_2$ | `KDEC` | Sander et al. (2019) |
| G42026 | TrGCN | $HOCH_2CHO$ + $NO_3$ → HOCH2CO + $HNO_3$ | `KNO3AL` | Rickard and Pascoe (2009) |
| G42027a | TrGC | $HOCH_2CO_3$ → HCHO + $CO_2$ + $HO_2$ | `k1_RO2RCO3*0.9` | Sander et al. (2019) |
| G42027b | TrGC | $HOCH_2CO_3$ → $HOCH_2CO_2H$ | `k1_RO2RCO3*0.1` | Sander et al. (2019) |
| G42028a | TrGC | $HOCH_2CO_3$ + $HO_2$ → HCHO + $HO_2$ + OH + $CO_2$ | `KAPHO2*r_CO3_OH` | Sander et al. (2019), Groß et al. (2014) |
| G42028b | TrGC | $HOCH_2CO_3$ + $HO_2$ → $HOCH_2CO_3H$ | `KAPHO2*r_CO3_OOH` | Sander et al. (2019), Groß et al. (2014) |
| G42028c | TrGC | $HOCH_2CO_3$ + $HO_2$ → $HOCH_2CO_2H$ + $O_3$ | `KAPHO2*r_CO3_O3` | Sander et al. (2019), Groß et al. (2014) |
| G42029 | TrGCN | $HOCH_2CO_3$ + NO → $NO_2$ + $HO_2$ + HCHO + $CO_2$ | `KAPNO` | Rickard and Pascoe (2009) |
| G42030 | TrGCN | $HOCH_2CO_3$ + $NO_2$ → PHAN | `k_CH3CO3_NO2` | Rickard and Pascoe (2009) |
| G42031 | TrGCN | $HOCH_2CO_3$ + $NO_3$ → $NO_2$ + $HO_2$ + HCHO + $CO_2$ | `KRO2NO3*1.74` | Rickard and Pascoe (2009) |
| G42032 | TrGC | $HOCH_2CO_2H$ + OH → .09 HCHO + .09 $CO_2$ + .91 $HCOCO_2H$ + $HO_2$ + $H_2O$ | `k_CO2H+k_s*f_sOH*f_CO2H` | Sander et al. (2019) |
| G42033a | TrGC | $HOCH_2CO_3H$ + OH → $HOCH_2CO_3$ + $H_2O$ | `k_ROOHRO` | Sander et al. (2019) |
| G42033b | TrGC | $HOCH_2CO_3H$ + OH → $HCOCO_3H$ + $HO_2$ | `k_s*f_sOH*f_CO2H` | Sander et al. (2019) |
| G42034 | TrGCN | PHAN → $HOCH_2CO_3$ + $NO_2$ | `k_PAN_M` | Rickard and Pascoe (2009) |
| G42035 | TrGCN | PHAN + OH → HCHO + CO + $NO_2$ + $H_2O$ | `k_s*f_sOH*f_cpan+k_ROHRO` | Sander et al. (2019) |
| G42036 | TrGC | GLYOX + OH → HCOCO + $H_2O$ | `3.1E-12*EXP(340./temp)` | Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013) |
| G42037 | TrGCN | GLYOX + $NO_3$ → HCOCO + $HNO_3$ | `KNO3AL` | Rickard and Pascoe (2009) |
| G42038a | TrGC | HCOCO → CO + CO + $HO_2$ | `7.E11*EXP(-3160./temp) +5.E-12*c(ind_O2)` | Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009) |
| G42037b | TrGC | HCOCO → $HCOCO_3$ | `5.E-12*c(ind_O2)*3.2*exp(-550./ temp)` | Lockhart et al. (2013), Rickard and Pascoe (2009) |
| G42037c | TrGC | HCOCO → OH + CO + $CO_2$ | `5.E-12*c(ind_O2) *(1.-3.2*exp(-550./temp))` | Lockhart et al. (2013), Rickard and Pascoe (2009) |
| G42039a | TrGC | $HCOCO_3$ → CO + $HO_2$ + $CO_2$ | `k1_RO2RCO3*0.9` | Sander et al. (2019) |
| G42039b | TrGC | $HCOCO_3$ → $HCOCO_2H$ | `k1_RO2RCO3*0.1` | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42040 | TrGC | $HCOCO_3 + HO_2 \rightarrow HO_2 + CO + CO_2 + OH$ | KAPHO2 | Feierabend et al. (2008), Sander et al. (2019) |
| G42041 | TrGCN | $HCOCO_3 + NO \rightarrow HO_2 + CO + NO_2 + CO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G42042 | TrGCN | $HCOCO_3 + NO_3 \rightarrow HO_2 + CO + NO_2 + CO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G42043 | TrGCN | $HCOCO_3 + NO_2 \rightarrow HO_2 + CO + NO_3 + CO_2$ | k_CH3CO3_NO2 | Orlando and Tyndall (2001), Sander et al. (2019) |
| G42044 | TrGC | $HCOCO_2H + OH \rightarrow CO + HO_2 + CO_2 + H_2O$ | k_CO2H+k_t*f_O*f_CO2H | Sander et al. (2019) |
| G42045a | TrGC | $HCOCO_3H + OH \rightarrow HCOCO_3 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G42045b | TrGC | $HCOCO_3H + OH \rightarrow CO + CO_2 + H_2O + OH$ | k_t*f_O*f_CO2H | Sander et al. (2019) |
| G42046 | TrGC | $HOCH_2CH_2O_2 \rightarrow .6\ HOCH_2CH_2O + .2\ HOCH_2CHO + .2$ ETHGLY | 2.*(7.8E-14*EXP(1000./temp) *k_CH3O2)**(.5)*RO2 | Atkinson et al. (2006), Rickard and Pascoe (2009) |
| G42047 | TrGCN | $HOCH_2CH_2O_2 + NO \rightarrow .25\ HO_2 + .5\ HCHO + .75\ HOCH_2CH_2O + NO_2$ | KRO2NO*(1.-alpha_AN(3,1,0,0,0, temp,cair)) | Rickard and Pascoe (2009)* |
| G42048 | TrGCN | $HOCH_2CH_2O_2 + NO \rightarrow$ ETHOHNO3 | KRO2NO*alpha_AN(3,1,0,0,0,temp, cair) | Sander et al. (2019) |
| G42049a | TrGC | $HOCH_2CH_2O_2 + HO_2 \rightarrow$ HYETHO2H | 1.53E-13*EXP(1300./temp) *(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G42049b | TrGC | $HOCH_2CH_2O_2 + HO_2 \rightarrow HOCH_2CH_2O + OH$ | 1.53E-13*EXP(1300./temp) *r_CHOHCH2O2_OH | Rickard and Pascoe (2009) |
| G42050 | TrGCN | ETHOHNO3 + OH $\rightarrow .93\ NO_3$CH2CHO $+ .93\ HO_2 + .07\ HOCH_2CHO + .07\ NO_2 + H_2O$ | k_s*(f_sOH*f_CH2ONO2+f_ONO2*f_ pCH2OH)+k_ROHRO | Sander et al. (2019) |
| G42051a | TrGC | HYETHO2H + OH $\rightarrow HOCH_2CH_2O_2 + H_2O$ | k_ROOHRO | Rickard and Pascoe (2009)* |
| G42051b | TrGC | HYETHO2H + OH $\rightarrow HOCH_2CHO + OH + H_2O$ | k_s*f_sOOH*f_pCH2OH | Sander et al. (2019) |
| G42051c | TrGC | HYETHO2H + OH $\rightarrow$ HOOCH2CHO $+ HO_2 + H_2O$ | k_s*f_sOH*f_pCH2OH+k_ROHRO | Sander et al. (2019) |
| G42052a | TrGC | $HOCH_2CH_2O \rightarrow HO_2 + HOCH_2CHO$ | 6.00E-14*EXP(-550./temp) *C(ind_O2) | Rickard and Pascoe (2009) |
| G42052b | TrGC | $HOCH_2CH_2O \rightarrow HO_2 + HCHO + HCHO$ | 9.50E13*EXP(-5988./temp) | Rickard and Pascoe (2009) |
| G42053 | TrGC | ETHGLY + OH $\rightarrow HOCH_2CHO + HO_2 + H_2O$ | 2.*k_s*f_sOH*f_pCH2OH+2.*k_ROHRO | Sander et al. (2019) |
| G42054 | TrGC | $HCOCH_2O_2 \rightarrow .6\ HCHO + .6\ CO + .6\ HO_2 + .2$ GLYOX $+ .2\ HOCH_2CHO$ | k1_RO2pORO2 | Sander et al. (2019) |
| G42055a | TrGC | $HCOCH_2O_2 + HO_2 \rightarrow$ HOOCH2CHO | k_RO2_HO2(temp,2)*r_COCH2O2_OOH | Sander et al. (2019) |
| G42055b | TrGC | $HCOCH_2O_2 + HO_2 \rightarrow HCHO + CO + HO_2 + OH$ | k_RO2_HO2(temp,2)*r_COCH2O2_OH | Sander et al. (2019) |
| G42056a | TrGCN | $HCOCH_2O_2 + NO \rightarrow NO_2 + HCHO + CO + HO_2$ | KRO2NO*(1.-alpha_AN(3,1,1,0,0, temp,cair)) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42056b | TrGCN | $HCOCH_2O_2$ + NO → $NO_3$CH2CHO | KRO2NO*alpha_AN(3,1,1,0,0,temp, cair) | Sander et al. (2019) |
| G42057 | TrGCN | $HCOCH_2O_2$ + $NO_3$ → HCHO + CO + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G42058a | TrGC | HOOCH2CHO + OH → $HCOCH_2O_2$ | k_ROOHRO | Sander et al. (2019) |
| G42058b | TrGC | HOOCH2CHO + OH → HCHO + CO + OH | 0.8*8.E-12 | Sander et al. (2019)* |
| G42058c | TrGC | HOOCH2CHO + OH → GLYOX + OH | k_s*f_sOOH*f_CHO | Sander et al. (2019) |
| G42059 | TrGCN | HOOCH2CHO + $NO_3$ → OH + HCHO + CO + $HNO_3$ | KNO3AL | Rickard and Pascoe (2009) |
| G42060 | TrGCN | $HOOCH_2CO_3$ + NO → $NO_2$ + OH + HCHO + $CO_2$ | KAPNO | Sander et al. (2019) |
| G42061 | TrGCN | $HOOCH_2CO_3$ + $NO_3$ → $NO_2$ + OH + HCHO + $CO_2$ | KRO2NO3*1.74 | Sander et al. (2019) |
| G42062a | TrGC | $HOOCH_2CO_3$ + $HO_2$ → 2 OH + HCHO + $CO_2$ | KAPHO2*r_CO3_OH | Sander et al. (2019) |
| G42062b | TrGC | $HOOCH_2CO_3$ + $HO_2$ → HOOCH2CO3H | KAPHO2*r_CO3_OOH | Sander et al. (2019) |
| G42062c | TrGC | $HOOCH_2CO_3$ + $HO_2$ → HOOCH2CO2H + $O_3$ | KAPHO2*r_CO3_O3 | Sander et al. (2019) |
| G42063a | TrGC | $HOOCH_2CO_3$ → OH + HCHO + $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G42063b | TrGC | $HOOCH_2CO_3$ → HOOCH2CO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G42064a | TrGC | HOOCH2CO3H + OH → $HOOCH_2CO_3$ + $H_2O$ | 2.*k_ROOHRO | Sander et al. (2019) |
| G42064b | TrGC | HOOCH2CO3H + OH → $HCOCO_3H$ + OH + $H_2O$ | k_s*f_sOOH*f_CO2H | Sander et al. (2019) |
| G42065 | TrGC | HOOCH2CO2H + OH → $HCOCO_2H$ + OH + $H_2O$ | k_s*f_sOOH*f_CO2H+k_CO2H | Sander et al. (2019) |
| G42066 | TrGC | CH2CO + OH → .6 HCHO + .6 $HO_2$ + .6 CO + .4 HOOCH2CO2H | 2.8E-12*exp(510./temp) | Baulch et al. (2005), Sander et al. (2019) |
| G42067a | TrGC | CH3CHOHOOH + OH → $CH_3COOH$ + OH | (k_t*f_tOOH*f_tOH + k_ROHRO) | Sander et al. (2019) |
| G42067b | TrGC | CH3CHOHOOH + OH → CH3CHOHO2 | k_ROOHRO | Sander et al. (2019) |
| G42068 | TrGC | CH3CHOHO2 → $CH_3CHO$ + $HO_2$ | 3.46E12*EXP(-12500./(1.98*temp)) | Hermans et al. (2005), Sander et al. (2019) |
| G42069 | TrGC | $CH_3CHO$ + $HO_2$ → CH3CHOHO2 | 3.46E12*EXP(-12500./(1.98*temp)) /(6.34E26*EXP(-14700./ (1.98*temp))) | Hermans et al. (2005), Sander et al. (2019) |
| G42070 | TrGC | CH3CHOHO2 + $HO_2$ → .5 CH3CHOHOOH + .3 $CH_3COOH$ + .2 $CH_3$ + .2 HCOOH + .2 OH | 5.6E-15*EXP(2300./temp) | Sander et al. (2019) |
| G42071 | TrGC | CH3CHOHO2 → $CH_3$ + HCOOH + OH | k1_RO2sORO2 | Sander et al. (2019) |
| G42072 | TrGCN | CH3CHOHO2 + NO → $CH_3$ + HCOOH + OH + $NO_2$ | KRO2NO | Sander et al. (2019) |
| G42073 | TrGCN | $C_2H_5ONO_2$ + OH → $CH_3CHO$ + $H_2O$ + $NO_2$ | 6.7E-13*EXP(-395./temp) | Atkinson et al. (2006) |
| G42074a | TrGCN | $NO_3$CH2CHO + OH → GLYOX + $NO_2$ + $H_2O$ | k_s*f_CH2ONO2*f_CHO | Paulot et al. (2009a), Sander et al. (2019)* |
| G42074b | TrGCN | $NO_3$CH2CHO + OH → $NO_3CH2CO_3$ + $H_2O$ | k_t*f_O*f_CH2ONO2*3. | Paulot et al. (2009a), Sander et al. (2019)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42075 | TrGCN | $NO_3CH2CO_3 + HO_2 \rightarrow HCHO + NO_2 + CO_2 + OH$ | `KAPHO2` | Rickard and Pascoe (2009)* |
| G42076 | TrGCN | $NO_3CH2CO_3 + NO \rightarrow HCHO + NO_2 + CO_2 + NO_2$ | `KAPNO` | Rickard and Pascoe (2009) |
| G42077 | TrGCN | $NO_3CH2CO_3 + NO_2 \rightarrow NO_3CH2CHO$ | `k_CH3CO3_NO2` | Rickard and Pascoe (2009) |
| G42078 | TrGCN | $NO_3CH2CO_3 \rightarrow HCHO + NO_2 + CO_2$ | `k1_RO2RCO3` | Rickard and Pascoe (2009)* |
| G42079 | TrGCN | $NO_3CH2CHO \rightarrow NO_3CH2CO_3 + NO_2$ | `k_PAN_M` | Rickard and Pascoe (2009) |
| G42080 | StTrGCN | $C_2H_5O_2 + NO_2 \rightarrow C_2H_5O_2NO_2$ | `k_3rd_iupac(temp,cair,1.3E-29, 6.2,8.8E-12,0.0,0.31)` | Atkinson et al. (2006) |
| G42081 | StTrGCN | $C_2H_5O_2NO_2 \rightarrow C_2H_5O_2 + NO_2$ | `k_3rd_iupac(temp,cair, REAL(4.8E-4*EXP(-9285./temp) ,SP),0.0,REAL(8.8E15*EXP(-10440./ temp),SP),0.0,0.31)` | Atkinson et al. (2006) |
| G42082 | StTrGCN | $C_2H_5O_2NO_2 + OH \rightarrow CH_3CHO + NO_3 + H_2O$ | `9.50E-13*EXP(-650./temp)` | Sander et al. (2019)* |
| G42083a | TrGC | $CH_3C(O) + O_2 \rightarrow CH_3C(O)OO$ | `5.1E-12*(1. - 1./(1.+ 9.4E-18*cair))` | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42083b | TrGC | $CH_3C(O) + O_2 \rightarrow OH + HCHO + CO$ | `5.1E-12*1./(1.+9.4E-18*cair)` | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42084 | TrGC | $C_2H_5OH + OH \rightarrow .95\ C_2H_5O_2 + .95\ HO_2 + .05\ HOCH_2CH_2O_2 + H_2O$ | `3.0E-12*EXP(20./temp)` | Sander et al. (2019), Atkinson et al. (2006) |
| G42085a | TrGCN | $CH_3CN + OH \rightarrow NCCH_2O_2 + H_2O$ | `8.1E-13*EXP(-1080./temp)*0.40` | Atkinson et al. (2006), Tyndall et al. (2001b)* |
| G42085b | TrGCN | $CH_3CN + OH \rightarrow OH + CH_3C(O) + NO$ | `8.1E-13*EXP(-1080./temp)*(1.-0.40)` | Atkinson et al. (2006), Tyndall et al. (2001b)* |
| G42086a | TrGCN | $CH_3CN + O(^1D) \rightarrow O(^3P) + CH_3CN$ | `2.54E-10*EXP(-24./temp) *0.0269*EXP(137./temp)` | Strekowski et al. (2010) |
| G42086b | TrGCN | $CH_3CN + O(^1D) \rightarrow 2\ H + CO + HCN$ | `2.54E-10*EXP(-24./temp)*0.16` | Strekowski et al. (2010)* |
| G42086c | TrGCN | $CH_3CN + O(^1D) \rightarrow .5\ CH_3 + .5\ NCO + .5\ NCCH_2O_2 + .5\ OH$ | `2.54E-10*EXP(-24./temp)*(1.-(0.16+ 0.0269*EXP(137./temp)))` | Strekowski et al. (2010)* |
| G42087 | TrGCN | $NCCH_2O_2 + NO \rightarrow HCN + CO_2 + HO_2 + NO_2$ | `KRO2NO` | see note* |
| G42088 | TrGCN | $NCCH_2O_2 + HO_2 \rightarrow HCN + CO_2 + HO_2$ | `k_RO2_HO2(temp,2)` | see note* |
| G42089a | TrGC | $CH_2CHOH + OH \rightarrow HCOOH + OH + HCHO$ | `k_CH2CHOH_OH_HCOOH` | Sander et al. (2019), So et al. (2014)* |
| G42089b | TrGC | $CH_2CHOH + OH \rightarrow HOCH_2CHO + HO_2$ | `k_CH2CHOH_OH_ALD` | Sander et al. (2019), So et al. (2014) |
| G42090 | TrGC | $CH_2CHOH + HCOOH \rightarrow CH_3CHO + HCOOH$ | `k_CH2CHOH_HCOOH` | Sander et al. (2019), da Silva (2010)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G42091 | TrGC | $CH_3CHO + HCOOH \rightarrow CH_2CHOH + HCOOH$ | k_ALD_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G42092 | TrGC | $HOOCCOOH + OH \rightarrow 2\ CO_2 + HO_2 + H_2O$ | 2.0 *k_co2h | see note* |
| G42093a | TrGC | $HOCH_2CHOHOH + OH \rightarrow HOCH_2CO_2H + HO_2 + H_2O$ | k_t*f_toh*f_toh | see note* |
| G42093b | TrGC | $HOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + HO_2 + H_2O$ | k_s*f_soh*f_pch2oh | see note* |
| G42093c | TrGC | $HOCH_2CHOHOH + OH \rightarrow HCOOH + HOCH_2O_2 + H_2O$ | 2.0 * k_rohro | see note* |
| G42093d | TrGC | $HOCH_2CHOHOH + OH \rightarrow HCHO + HCOOH + HO_2 + H_2O$ | k_rohro | see note* |
| G42094a | TrGC | $CH_3CHOHOH + OH \rightarrow CH_3COOH + HO_2 + H_2O$ | k_t*f_toh*f_toh | see note* |
| G42094b | TrGC | $CH_3CHOHOH + OH \rightarrow CH_3 + HCOOH + H_2O$ | 2.0 * k_rohro | see note* |
| G42095a | TrGC | $CHOHOHCOOH + OH \rightarrow HOOCCOOH + HO_2 + H_2O$ | k_t*f_toh*f_toh*f_co2h | see note* |
| G42095b | TrGC | $CHOHOHCOOH + OH \rightarrow HCOOH + CO_2 + HO_2 + H_2O$ | 2.0 * k_rohro + k_co2h | see note* |
| G42096a | TrGC | $CHOHOHCHOHOH + OH \rightarrow 2\ HCOOH + HO_2 + H_2O$ | 4.0 * k_rohro | see note* |
| G42096b | TrGC | $CHOHOHCHOHOH + OH \rightarrow CHOHOHCOOH + HO_2 + H_2O$ | 2.0 * k_t*f_toh*f_toh*f_pch2oh | see note* |
| G42097a | TrGC | $CHOCHOHOH + OH \rightarrow HCOOH + CO + HO_2 + H_2O$ | 2.0 * k_rohro + k_t*f_o*f_pch2oh | see note* |
| G42097b | TrGC | $CHOCHOHOH + OH \rightarrow HCOCO_2H + HO_2 + H_2O$ | k_t*f_toh*f_toh*f_cho | see note* |
| G42098a | TrGC | $HOOCH_2CHOHOH + OH \rightarrow$ HOOCH2CO2H $+ HO_2 + H_2O$ | k_t*f_toh*f_toh*f_pch2oh | see note* |
| G42098b | TrGC | $HOOCH_2CHOHOH + OH \rightarrow HCOOH + HCHO + OH + H_2O$ | 2.0 * k_rohro | see note* |
| G42098c | TrGC | $HOOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + OH + H_2O$ | k_s*f_pch2oh*f_sooh | see note* |
| G43000a | TrGC | $C_3H_8 + OH \rightarrow iC_3H_7O_2 + H_2O$ | k_s | Sander et al. (2019) |
| G43000b | TrGC | $C_3H_8 + OH \rightarrow C_3H_7O_2 + H_2O$ | 2.*k_p | Sander et al. (2019) |
| G43001a | TrGC | $C_3H_6 + O_3 \rightarrow HCHO + .16$ CH3CHOHOOH $+ .50\ OH + .50\ HCOCH_2O_2 + .05$ CH2CO $+ .09\ CH_3OH + .09\ CO + .2\ CH_4 + .2\ CO_2$ | 5.5E-15*EXP(-1880./temp)*.57 | Atkinson et al. (2006)* |
| G43001b | TrGC | $C_3H_6 + O_3 \rightarrow CH_3CHO + CH_2OO^*$ | 5.5E-15*EXP(-1880./temp)*.43 | Atkinson et al. (2006)* |
| G43002 | TrGC | $C_3H_6 + OH \rightarrow$ HYPROPO2 | k_3rd_iupac(temp,cair,8.6E-27, 3.5,3.E-11,1.,0.5) | Atkinson et al. (2006), Rickard and Pascoe (2009) |
| G43003 | TrGCN | $C_3H_6 + NO_3 \rightarrow$ PRONO3BO2 | 4.6E-13*EXP(-1155./temp) | Wallington et al. (2018) |
| G43004 | TrGC | $iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$ | 1.9E-13*EXP(1300./temp) | Atkinson (1997)* |
| G43005a | TrGCN | $iC_3H_7O_2 + NO \rightarrow CH_3COCH_3 + HO_2 + NO_2$ | 2.7E-12*EXP(360./temp)*(1.-alpha_ AN(3,2,0,0,0,temp,cair)) | Wallington et al. (2018) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G43005b | TrGCN | $iC_3H_7O_2 + NO \rightarrow iC_3H_7ONO_2$ | 2.7E-12*EXP(360./temp)*alpha_AN(3,2,0,0,0,temp,cair) | Wallington et al. (2018) |
| G43006 | TrGC | $iC_3H_7O_2 \rightarrow .8\ CH_3COCH_3 + .2$ IPROPOL $+ .6\ HO_2$ | 2.*(1.6E-12*EXP(-2200./temp)*k_CH3O2)**(.5)*RO2 | Rickard and Pascoe (2009), Atkinson et al. (2006) |
| G43007a | TrGC | $iC_3H_7OOH + OH \rightarrow iC_3H_7O_2 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G43007b | TrGC | $iC_3H_7OOH + OH \rightarrow CH_3COCH_3 + H_2O + OH$ | k_t*f_tOOH | Sander et al. (2019) |
| G43008 | TrGC | $C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$ | 1.9E-13*EXP(1300./temp) | Atkinson (1997)* |
| G43009a | TrGCN | $C_3H_7O_2 + NO \rightarrow C_2H_5CHO + HO_2 + NO_2$ | 2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,1,0,0,0,temp,cair)) | Wallington et al. (2018) |
| G43009b | TrGCN | $C_3H_7O_2 + NO \rightarrow C_3H_7ONO_2$ | 2.7E-12*EXP(360./temp)*alpha_AN(3,1,0,0,0,temp,cair) | Wallington et al. (2018) |
| G43010 | TrGC | $C_3H_7O_2 \rightarrow .8\ CH_3COCH_3 + .2$ NPROPOL $+ .6\ HO_2$ | 2.*(k_CH3O2*3.E-13)**(.5)*RO2 | Rickard and Pascoe (2009), Atkinson et al. (2006) |
| G43011 | TrGC | $CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$ | (8.8E-12*EXP(-1320./temp)+1.7E-14*EXP(423./temp)) | Atkinson et al. (2006)* |
| G43012a | TrGC | $CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$ | 8.6E-13*EXP(700./temp)*r_COCH2O2_OOH | Tyndall et al. (2001a), Sander et al. (2019) |
| G43012b | TrGC | $CH_3COCH_2O_2 + HO_2 \rightarrow OH + CH_3C(O) + HCHO$ | 8.6E-13*EXP(700./temp)*r_COCH2O2_OH | Tyndall et al. (2001a), Sander et al. (2019) |
| G43013a | TrGCN | $CH_3COCH_2O_2 + NO \rightarrow CH_3C(O) + HCHO + NO_2$ | 2.9E-12*EXP(300./temp)*(1.-alpha_AN(4,1,1,0,0,temp,cair)) | Burkholder et al. (2015) |
| G43013b | TrGCN | $CH_3COCH_2O_2 + NO \rightarrow$ NOA | 2.9E-12*EXP(300./temp)*alpha_AN(4,1,1,0,0,temp,cair) | Burkholder et al. (2015) |
| G43014 | TrGC | $CH_3COCH_2O_2 \rightarrow .3\ CH_3C(O) + .3\ HCHO + .5$ MGLYOX $+ .2\ CH_3COCH_2OH$ | k1_RO2pORO2 | Orlando and Tyndall (2012) |
| G43015a | TrGC | $CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2 + H_2O$ | k_ROOHRO | see note* |
| G43015b | TrGC | $CH_3COCH_2O_2H + OH \rightarrow$ MGLYOX $+ OH + H_2O$ | k_s*f_sOOH*f_CO | Sander et al. (2019) |
| G43016 | TrGC | $CH_3COCH_2OH + OH \rightarrow$ MGLYOX $+ HO_2 + H_2O$ | 1.6E-12*EXP(305./temp) | Atkinson et al. (2006) |
| G43017 | TrGC | MGLYOX $+ OH \rightarrow .4\ CH_3 + .6\ CH_3C(O) + 1.4\ CO + H_2O$ | 1.9E-12*EXP(575./temp) | Baeza-Romero et al. (2007), Atkinson et al. (2006) |
| G43020 | TrGCN | $iC_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$ | 6.2E-13*EXP(-230./temp) | Wallington et al. (2018) |
| G43021 | TrGCN | $CH_3COCH_2O_2 + NO_3 \rightarrow CH_3C(O) + HCHO + NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G43022 | TrGC | HYPROPO2 $\rightarrow CH_3CHO + HCHO + HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G43023a | TrGC | HYPROPO2 $+ HO_2 \rightarrow$ HYPROPO2H | k_RO2_HO2(temp,3)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G43023b | TrGC | HYPROPO2 + $HO_2$ → $CH_3CHO$ + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,3)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009) |
| G43024a | TrGCN | HYPROPO2 + NO → $CH_3CHO$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(4,1,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G43024b | TrGCN | HYPROPO2 + NO → PROPOLNO3 | KRO2NO*alpha_AN(4,1,0,0,0,temp, cair) | Rickard and Pascoe (2009) |
| G43025 | TrGCN | HYPROPO2 + $NO_3$ → $CH_3CHO$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G43026a | TrGC | HYPROPO2H + OH → HYPROPO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G43026b | TrGC | HYPROPO2H + OH → $CH_3COCH_2OH$ + OH | (k_s*f_sOH*f_pCH2OH+k_t*f_ tOOH*f_pCH2OH) | Sander et al. (2019) |
| G43027 | TrGCN | PRONO3BO2 + $HO_2$ → PR2O2HNO3 | k_RO2_HO2(temp,3) | Rickard and Pascoe (2009) |
| G43028 | TrGCN | PRONO3BO2 + NO → NOA + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G43029 | TrGCN | PRONO3BO2 + $NO_3$ → NOA + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G43030a | TrGCN | PR2O2HNO3 + OH → PRONO3BO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G43030b | TrGCN | PR2O2HNO3 + OH → NOA + OH | k_t*f_tOOH*f_CH2ONO2 | Sander et al. (2019) |
| G43031 | TrGCN | MGLYOX + $NO_3$ → $CH_3C(O)$ + CO + $HNO_3$ | KNO3AL*2.4 | Rickard and Pascoe (2009) |
| G43032 | TrGCN | NOA + OH → MGLYOX + $NO_2$ | (k_s*f_CO*f_ONO2+k_p*f_CO) | Sander et al. (2019) |
| G43033 | TrGC | HOCH2COCHO + OH → .8609 HOCH2CO + .8609 CO + .1391 HCOCOCHO + .1391 $HO_2$ | (1.9E-12*EXP(575./temp)+k_s*f_ sOH*f_CO) | Sander et al. (2019) |
| G43034 | TrGCN | HOCH2COCHO + $NO_3$ → HOCH2CO + CO + $HNO_3$ | KNO3AL*2.4 | Sander et al. (2019) |
| G43035 | TrGC | $CH_3COCO_2H$ + OH → $CH_3C(O)$ + $H_2O$ + $CO_2$ | 4.9E-14*EXP(276./temp) | Mellouki and Mu (2003), Sander et al. (2019) |
| G43036 | TrGC | $HCOCOCH_2O_2$ → .6 HCOCO + .6 HCHO + .2 HCOCOCHO + .2 HOCH2COCHO | k1_RO2pORO2 | Sander et al. (2019) |
| G43037 | TrGCN | $HCOCOCH_2O_2$ + NO → HCOCO + HCHO + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G43038a | TrGC | $HCOCOCH_2O_2$ + $HO_2$ → $HCOCOCH_2OOH$ | k_RO2_HO2(temp,3)*r_COCH2O2_OOH | Sander et al. (2019) |
| G43038b | TrGC | $HCOCOCH_2O_2$ + $HO_2$ → HCOCO + HCHO + OH | k_RO2_HO2(temp,3)*r_COCH2O2_OH | Sander et al. (2019) |
| G43039 | TrGCN | $HCOCOCH_2O_2$ + $NO_3$ → HCOCO + HCHO + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G43040a | TrGC | $HCOCOCH_2OOH$ + OH → $HOOCH_2CO_3$ + CO + $H_2O$ | k_t*f_CO*f_O | Sander et al. (2019)* |
| G43040b | TrGC | $HCOCOCH_2OOH$ + OH → HCOCOCHO + $H_2O$ + OH | k_s*f_sOOH*f_CO | Sander et al. (2019)* |
| G43040c | TrGC | $HCOCOCH_2OOH$ + OH → $HCOCOCH_2O_2$ + $H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G43041 | TrGCN | $HCOCOCH_2OOH$ + $NO_3$ → $HOOCH_2CO_3$ + CO + $HNO_3$ | KNO3AL*2.4 | Sander et al. (2019) |
| G43042 | TrGC | HOCH2COCH2O2 → HCHO + HOCH2CO | k1_RO2pORO2 | Sander et al. (2019) |
| G43043a | TrGC | HOCH2COCH2O2 + $HO_2$ → HOCH2COCH2OOH | k_RO2_HO2(temp,3)*r_COCH2O2_OOH | Sander et al. (2019) |
| G43043b | TrGC | HOCH2COCH2O2 + $HO_2$ → HCHO + HOCH2CO + OH | k_RO2_HO2(temp,3)*r_COCH2O2_OH | Sander et al. (2019) |
| G43044 | TrGCN | HOCH2COCH2O2 + NO → HCHO + HOCH2CO + $NO_2$ | KRO2NO | Sander et al. (2019)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G43045a | TrGC | HOCH2COCH2OOH + OH → HOCH2COCHO + OH | k_s*f_sOOH*f_CO | Sander et al. (2019) |
| G43045b | TrGC | HOCH2COCH2OOH + OH → HOCH2COCH2O2 | k_ROOHRO | Sander et al. (2019) |
| G43045c | TrGC | HOCH2COCH2OOH + OH → $HCOCOCH_2OOH + HO_2$ | 1.60E-12*EXP(305./temp) | Sander et al. (2019)* |
| G43046 | TrGC | CH3CHCO + OH → .72 CO + .72 $CH_3CHO$ + .72 $HO_2$ + .21 $CH_3COCO_2H$ + .07 $CH_3CHO$ + .07 $HO_2$ + .07 $CO_2$ | 7.6E-11 | Hatakeyama et al. (1985), Sander et al. (2019) |
| G43047 | TrGCN | PROPOLNO3 + OH → $CH_3COCH_2OH + NO_2$ | k_t*f_ONO2*f_pCH2OH+k_s*f_sOH*f_CH2ONO2 | Sander et al. (2019) |
| G43048 | TrGCN | $CH_3COCH_2O_2 + NO_2 \rightarrow CH_3COCH_2OONO_2$ | 2.3E-12*EXP(300./temp) | Tyndall et al. (2001a)* |
| G43049 | TrGCN | $CH_3COCH_2OONO_2 \rightarrow CH_3COCH_2O_2 + NO_2$ | 1.9E16*EXP(-10830./temp) | Sehested et al. (1998)* |
| G43050 | TrGCN | $CH_3COCH_2OONO_2$ + OH → MGLYOX + $NO_3 + H_2O$ | 9.50E-13*EXP(-650./temp)*f_CO | Sander et al. (2019)* |
| G43051a | TrGC | $C_3H_7OOH + OH \rightarrow C_3H_7O_2 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G43051b | TrGC | $C_3H_7OOH + OH \rightarrow C_2H_5CHO + H_2O + OH$ | k_s*f_sOOH | Sander et al. (2019) |
| G43051c | TrGC | $C_3H_7OOH + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$ | k_s*f_pCH2OH | Sander et al. (2019)* |
| G43052 | TrGC | $C_2H_5CHO + OH \rightarrow C_2H_5CO_3 + H_2O$ | 4.9E-12*EXP(405./temp) | Atkinson et al. (2006)* |
| G43053 | TrGCN | $C_2H_5CHO + NO_3 \rightarrow C_2H_5CO_3 + HNO_3$ | 6.3E-15 | Atkinson et al. (2006) |
| G43054a | TrGC | $C_2H_5CO_3 \rightarrow C_2H_5O_2 + CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G43054b | TrGC | $C_2H_5CO_3 \rightarrow C_2H_5CO_2H$ | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G43055a | TrGC | $C_2H_5CO_3 + HO_2 \rightarrow C_2H_5O_2 + CO_2 + OH$ | KAPHO2*r_CO3_OH | Sander et al. (2019), Groß et al. (2014) |
| G43055b | TrGC | $C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_3H$ | KAPHO2*r_CO3_OOH | Sander et al. (2019), Groß et al. (2014) |
| G43055c | TrGC | $C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_2H + O_3$ | KAPHO2*r_CO3_O3 | Sander et al. (2019), Groß et al. (2014) |
| G43056 | TrGCN | $C_2H_5CO_3 + NO \rightarrow NO_2 + C_2H_5O_2 + CO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43057 | TrGCN | $C_2H_5CO_3 + NO_2$ → PPN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43058 | TrGCN | PPN → $C_2H_5CO_3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43059 | TrGC | $C_2H_5CO_2H + OH \rightarrow CH_3CHO + CO_2 + H_2O$ | k_CO2H+k_p+k_s*f_CO2H | Sander et al. (2019)* |
| G43060a | TrGC | $C_2H_5CO_3H + OH \rightarrow C_2H_5CO_3 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G43060b | TrGC | $C_2H_5CO_3H + OH \rightarrow CH_3CHO + CO_2 + H_2O$ | k_s*f_CO2H+k_p | Sander et al. (2019)* |
| G43061 | TrGCN | PPN + OH → $CH_3CHO + CO_2 + NO_2 + H_2O$ | k_s*f_cpan+k_p | Sander et al. (2019)* |
| G43062 | TrGC | $CH_3COCO_3H + OH \rightarrow CH_3COCO_3 + H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G43063a | TrGC | $CH_3COCO_3 + HO_2 \rightarrow CH_3C(O) + CO_2 + OH$ | KAPHO2*r_CO3_OH | Sander et al. (2019) |
| G43063b | TrGC | $CH_3COCO_3 + HO_2 \rightarrow CH_3COCO_3H$ | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Sander et al. (2019) |
| G43064 | TrGCN | $CH_3COCO_3 + NO \rightarrow CH_3C(O) + CO_2 + NO_2$ | KAPNO | Sander et al. (2019) |
| G43065 | TrGCN | $CH_3COCO_3 + NO_2 \rightarrow CH_3C(O) + CO_2 + NO_3$ | k_CH3CO3_NO2 | Sander et al. (2019)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G43066 | TrGCN | $CH_3COCO_3 + NO_3 \rightarrow CH_3C(O)OO + CO_2 + NO_2$ | KRO2NO3*1.74 | Sander et al. (2019) |
| G43067 | TrGC | $CH_3COCO_3 \rightarrow CH_3C(O)OO + CO_2$ | k1_RO2RCO3 | Sander et al. (2019) |
| G43068 | TrGC | $HCOCOCHO + OH \rightarrow 3\ CO + HO_2$ | 2.*k_t*f_CO*f_O | Sander et al. (2019) |
| G43069 | TrGC | $IPROPOL + OH \rightarrow CH_3COCH_3 + HO_2 + H_2O$ | 2.6E-12*EXP(200./temp) | Atkinson et al. (2006) |
| G43070a | TrGC | $NPROPOL + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$ | 4.6E-12*EXP(70./temp)*(k_s*f_sOH/(k_p+k_s*f_pCH2OH+k_s*f_sOH)) | Atkinson et al. (2006), Sander et al. (2019)* |
| G43070b | TrGC | $NPROPOL + OH \rightarrow HYPROPO2 + H_2O$ | 4.6E-12*EXP(70./temp)*((k_p+k_s*f_pCH2OH)/(k_p+k_s*f_pCH2OH+k_s*f_sOH)) | Atkinson et al. (2006), Sander et al. (2019)* |
| G43071a | TrGC | $CH_2CHCH_2OH + OH \rightarrow HCOOH + OH + CH_3CHO$ | k_CH2CHOH_OH_HCOOH | Sander et al. (2019), So et al. (2014)* |
| G43072 | TrGC | $CH_2CHCH_2OH + HCOOH \rightarrow C_2H_5CHO + HCOOH$ | k_CH2CHOH_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G43073 | TrGC | $C_2H_5CHO + HCOOH \rightarrow CH_2CHCH_2OH + HCOOH$ | k_ALD_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G43074 | TrGC | $HCOCOCH_2OOH + OH \rightarrow HCOCO + CO + HO_2 + OH$ | k_s*f_sOOH*f_CO+k_ROOHRO | Sander et al. (2019)* |
| G43075a | TrGC | $CH_3COCHOHOH + OH \rightarrow CH_3C(O) + HCOOH + H_2O$ | 2.0 * k_rohro | see note* |
| G43075b | TrGC | $CH_3COCHOHOH + OH \rightarrow CH_3COCO_2H + H_2O$ | k_t*f_toh*f_toh*f_co | see note* |
| G43202 | TrGTerC | HCOCH2CHO + OH → HCOCH2CO3 | 4.29E-11 | Rickard and Pascoe (2009) |
| G43203 | TrGTerCN | HCOCH2CHO + $NO_3$ → HCOCH2CO3 + $HNO_3$ | 2.*KNO3AL*2.4 | Rickard and Pascoe (2009) |
| G43204a | TrGTerC | HCOCH2CO3 → $HCOCH_2O_2 + CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G43204b | TrGTerC | HCOCH2CO3 → HCOCH2CO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G43205 | TrGTerCN | HCOCH2CO3 + NO → $HCOCH_2O_2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43206 | TrGTerCN | HCOCH2CO3 + $NO_2$ → $C_3PAN2$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43207a | TrGTerC | HCOCH2CO3 + $HO_2$ → HCOCH2CO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G43207b | TrGTerC | HCOCH2CO3 + $HO_2$ → HCOCH2CO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G43207c | TrGTerC | HCOCH2CO3 + $HO_2$ → $HCOCH_2O_2 + CO_2 + OH$ | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G43210 | TrGTerCN | $C_3PAN2$ → HCOCH2CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43211 | TrGTerCN | $C_3PAN2 + OH \rightarrow GLYOX + CO + NO_2$ | 2.10E-11 | Rickard and Pascoe (2009) |
| G43212 | TrGTerC | HCOCH2CO2H + OH → $HCOCH_2O_2 + CO_2$ | 2.14E-11 | Rickard and Pascoe (2009) |
| G43213a | TrGTerC | $HOC_2H_4CO_3 \rightarrow HOCH_2CH_2O_2 + CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G43213b | TrGTerC | $HOC_2H_4CO_3$ → HOC2H4CO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G43214 | TrGTerCN | $HOC_2H_4CO_3 + NO \rightarrow HOCH_2CH_2O_2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43215a | TrGTerC | $HOC_2H_4CO_3 + HO_2$ → HOC2H4CO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G43215b | TrGTerC | $HOC_2H_4CO_3 + HO_2 \rightarrow HOCH_2CH_2O_2 + CO_2 + OH$ | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G43215c | TrGTerC | $HOC_2H_4CO_3$ + $HO_2$ → HOC2H4CO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G43218 | TrGTerCN | $HOC_2H_4CO_3$ + $NO_2$ → $C_3$PAN1 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43219 | TrGTerC | HOC2H4CO2H + OH → $HOCH_2CH_2O_2$ + $CO_2$ | 1.39E-11 | Rickard and Pascoe (2009) |
| G43220 | TrGTerC | HOC2H4CO3H + OH → $HOC_2H_4CO_3$ | 1.73E-11 | Rickard and Pascoe (2009) |
| G43221 | TrGTerCN | $C_3$PAN1 → $HOC_2H_4CO_3$ + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43222 | TrGTerCN | $C_3$PAN1 + OH → $HOCH_2CHO$ + CO + $NO_2$ | 4.51E-12 | Rickard and Pascoe (2009) |
| G43223 | TrGTerC | HCOCH2CO3H + OH → $HCOCH_2O_2$ + $CO_2$ + $H_2O$ | 2.49E-11 | Rickard and Pascoe (2009)* |
| G43415 | TrGAroC | C3DIALOOH + OH → HCOCOCHO + OH | 1.44E-10 | Rickard and Pascoe (2009) |
| G43418a | TrGAroC | C3DIALO2 + $HO_2$ → C3DIALOOH | k_RO2_HO2(temp,3)*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G43418b | TrGAroC | C3DIALO2 + $HO_2$ → GLYOX + CO + $HO_2$ + OH | k_RO2_HO2(temp,3)*r_CO3_OH | Rickard and Pascoe (2009) |
| G43419 | TrGAroCN | C3DIALO2 + NO → GLYOX + CO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G43420 | TrGAroCN | C3DIALO2 + $NO_3$ → GLYOX + CO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G43421 | TrGAroC | C3DIALO2 → GLYOX + CO + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G43422a | TrGAroC | HCOCOHCO3 + $HO_2$ → GLYOX + $CO_2$ + $HO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G43422b | TrGAroC | HCOCOHCO3 + $HO_2$ → HCOCOHCO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G43424 | TrGAroCN | HCOCOHCO3 + NO → GLYOX + $CO_2$ + $HO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43425 | TrGAroCN | HCOCOHCO3 + $NO_2$ → HCOCOHPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43426 | TrGAroCN | HCOCOHCO3 + $NO_3$ → GLYOX + $CO_2$ + $HO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G43427 | TrGAroC | HCOCOHCO3 → GLYOX + $CO_2$ + $HO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G43428 | TrGAroC | METACETHO + OH → $CH_3C(O)$ + $CO_2$ | 9.82E-11 | Rickard and Pascoe (2009) |
| G43442 | TrGAroCN | HCOCOHPAN + OH → GLYOX + CO + $NO_2$ | 6.97E-11 | Rickard and Pascoe (2009) |
| G43443 | TrGAroCN | HCOCOHPAN → HCOCOHCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43444 | TrGAroC | C32OH13CO + OH → HCOCOHCO3 | 1.36E-10 | Rickard and Pascoe (2009) |
| G43446 | TrGAroC | HCOCOHCO3H + OH → HCOCOHCO3 | 7.33E-11 | Rickard and Pascoe (2009) |
| G44000 | TrGC | $C_4H_{10}$ + OH → $LC_4H_9O_2$ + $H_2O$ | 2.03E-17*temp*temp*EXP(78./temp) | Atkinson et al. (2006)* |
| G44001a | TrGC | $LC_4H_9O_2$ → $C_3H_7CHO$ + $HO_2$ | (k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.1273 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44001b | TrGC | $LC_4H_9O_2$ → .636 MEK + .636 $HO_2$ + .364 $CH_3CHO$ + .364 $C_2H_5O_2$ | (k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.8727 | Rickard and Pascoe (2009), Sander et al. (2019)* |
| G44002 | TrGC | $LC_4H_9O_2$ + $HO_2$ → $LC_4H_9OOH$ | k_RO2_HO2(temp,4) | Rickard and Pascoe (2009) |
| G44003a | TrGCN | $LC_4H_9O_2$ + NO → $NO_2$ + $C_3H_7CHO$ + $HO_2$ | KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.1273 | Rickard and Pascoe (2009), Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44003b | TrGCN | $LC_4H_9O_2$ + NO → $NO_2$ + .636 MEK + .636 $HO_2$ + .364 $CH_3CHO$ + .364 $C_2H_5O_2$ | `KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.8727` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44003c | TrGCN | $LC_4H_9O_2$ + NO → LC4H9NO3 | `KRO2NO*(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair))` | Rickard and Pascoe (2009)* |
| G44004a | TrGCN | $LC_4H_9O_2$ + $NO_3$ → $NO_2$ + $C_3H_7CHO$ + $HO_2$ | `KRO2NO3*0.1273` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44004b | TrGCN | $LC_4H_9O_2$ + $NO_3$ → $NO_2$ + .636 MEK + .636 $HO_2$ + .364 $CH_3CHO$ + .364 $C_2H_5O_2$ | `KRO2NO3*0.8727` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44005a | TrGC | $LC_4H_9OOH$ + OH → $LC_4H_9O_2$ + $H_2O$ | `k_ROOHRO` | Sander et al. (2019) |
| G44005b | TrGC | $LC_4H_9OOH$ + OH → $C_3H_7CHO$ + $H_2O$ + OH | `k_s*f_tOOH*f_alk*(k_p/(k_p+k_s))` | Sander et al. (2019) |
| G44005c | TrGC | $LC_4H_9OOH$ + OH → MEK + $H_2O$ + OH | `k_t*f_tOOH*f_alk*(k_s/(k_p+k_s))` | Sander et al. (2019) |
| G44006a | TrGC | $iC_4H_{10}$ + OH → $TC_4H_9O_2$ + $H_2O$ | `1.17E-17*temp*temp*EXP(213./temp)*k_t/(3.*k_p+k_t)` | Atkinson (2003) |
| G44006b | TrGC | $iC_4H_{10}$ + OH → $IC_4H_9O_2$ + $H_2O$ | `1.17E-17*temp*temp*EXP(213./temp)*3.*k_p/(3.*k_p+k_t)` | Atkinson (2003) |
| G44007 | TrGC | $TC_4H_9O_2$ → $CH_3COCH_3$ + $CH_3$ | `k1_RO2tRO2` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44008 | TrGC | $TC_4H_9O_2$ + $HO_2$ → $TC_4H_9OOH$ | `k_RO2_HO2(temp,4)` | Rickard and Pascoe (2009) |
| G44009a | TrGCN | $TC_4H_9O_2$ + NO → $NO_2$ + $CH_3COCH_3$ + $CH_3$ | `KRO2NO*(1.-alpha_AN(4,3,0,0,0,temp,cair))` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44009b | TrGCN | $TC_4H_9O_2$ + NO → TC4H9NO3 | `KRO2NO*alpha_AN(4,3,0,0,0,temp,cair)` | Rickard and Pascoe (2009) |
| G44010a | TrGC | $TC_4H_9OOH$ + OH → $TC_4H_9O_2$ + $H_2O$ | `k_ROOHRO` | Sander et al. (2019) |
| G44010b | TrGC | $TC_4H_9OOH$ + OH → $CH_3COCH_3$ + HCHO + OH + $H_2O$ | `3.*k_p*f_tCH2OH` | Sander et al. (2019)* |
| G44011 | TrGCN | TC4H9NO3 + OH → $CH_3COCH_3$ + HCHO + $NO_2$ + $H_2O$ | `3.*k_p*f_CH2ONO2` | Sander et al. (2019)* |
| G44012 | TrGC | $IC_4H_9O_2$ → IPRCHO | `k1_RO2sRO2` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44013 | TrGC | $IC_4H_9O_2$ + $HO_2$ → $IC_4H_9OOH$ | `k_RO2_HO2(temp,4)` | Rickard and Pascoe (2009) |
| G44014a | TrGCN | $IC_4H_9O_2$ + NO → $NO_2$ + IPRCHO | `KRO2NO*(1.-alpha_AN(4,2,0,0,0,temp,cair))` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44014b | TrGCN | $IC_4H_9O_2$ + NO → IC4H9NO3 | `KRO2NO*alpha_AN(4,2,0,0,0,temp,cair)` | Rickard and Pascoe (2009) |
| G44015a | TrGC | $IC_4H_9OOH$ + OH → $IC_4H_9O_2$ + $H_2O$ | `k_ROOHRO` | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44015b | TrGC | $IC_4H_9OOH$ + OH → IPRCHO + OH + $H_2O$ | k_s*f_sOOH+2.*k_s+k_t*f_pCH2OH | Sander et al. (2019)* |
| G44016 | TrGCN | IC4H9NO3 + OH → IPRCHO + $NO_2$ + $H_2O$ | k_s*f_ONO2+2.*k_p+k_t*f_CH2ONO2 | Sander et al. (2019)* |
| G44017 | TrGC | MVK + $O_3$ → .87 MGLYOX + .5481 CO + .1392 $HO_2$ + .1392 OH + .3219 $CH_2OO$ + .13 HCHO + .04680 OH + .04680 CO + .07280 $CH_3C(O)$ + .026 $CH_3CHO$ + .026 $CO_2$ + .026 HCHO + .026 $HO_2$ + .02402 MGLYOX + .02402 $H_2O_2$ + .00718 $CH_3COCO_2H$ | 8.5E-16*EXP(-1520./temp) | Sander et al. (2019) |
| G44018 | TrGC | MVK + OH → LHMVKABO2 | 2.6E-12*EXP(610./temp) | Sander et al. (2019), Atkinson et al. (2006)* |
| G44019 | TrGC | MEK + OH → LMEKO2 + $H_2O$ | 1.5E-12*EXP(-90./temp) | Atkinson et al. (2006), Sander et al. (2019)* |
| G44020 | TrGC | LMEKO2 + $HO_2$ → LMEKOOH | k_RO2_HO2(temp,4) | Sander et al. (2019) |
| G44021a | TrGCN | LMEKO2 + NO → .62 $CH_3CHO$ + .62 $CH_3C(O)$ + .38 HCHO + .38 $CO_2$ + .38 $HOCH_2CH_2O_2$ + $NO_2$ | KRO2NO*(1.-(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair))) | Sander et al. (2019)* |
| G44021b | TrGCN | LMEKO2 + NO → LMEKNO3 | KRO2NO*(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair)) | Sander et al. (2019) |
| G44022a | TrGC | LMEKOOH + OH → LMEKO2 + $H_2O$ | k_ROOHRO | Sander et al. (2019) |
| G44022b | TrGC | LMEKOOH + OH → .62 BIACET + .38 HCHO + .38 $CO_2$ + .38 $HOCH_2CH_2O_2$ + $H_2O$ + OH | (.62*k_t*f_tOOH*f_CO+.38*k_s*f_sOOH) | Sander et al. (2019) |
| G44023a | TrGCN | LC4H9NO3 + OH → MEK + $NO_2$ + $H_2O$ | (k_t*f_ONO2*f_alk+k_p*f_alk+k_s*f_CH2ONO2+k_p)*(k_s/(k_p+k_s)) | Sander et al. (2019)* |
| G44023b | TrGCN | LC4H9NO3 + OH → $C_3H_7CHO$ + $NO_2$ + $H_2O$ | (k_p+k_s*(1.+f_CH2ONO2+f_ONO2)*f_alk)*(k_p/(k_p+k_s)) | Sander et al. (2019)* |
| G44024 | TrGCN | MPAN + OH → $CH_3COCH_2OH$ + CO + $NO_2$ | 3.2E-11 | Orlando et al. (2002) |
| G44025 | TrGCN | MPAN → MACO3 + $NO_2$ | k_PAN_M | see note* |
| G44026 | TrGC | LMEKO2 → .538 HCHO + .538 $CO_2$ + .459 $HOCH_2CH_2O_2$ + .079 $C_2H_5O_2$ + .462 $CH_3C(O)$ + .462 $CH_3CHO$ | (.62*k1_RO2sORO2+.38*k1_RO2pORO2) | Rickard and Pascoe (2009)* |
| G44027 | TrGC | MACR + OH → .45 MACO3 + .55 MACRO2 | 8.E-12*EXP(380./temp) | Orlando et al. (1999b), Sander et al. (2019) |
| G44028 | TrGC | MACR + $O_3$ → .5481 CO + .1392 $HO_2$ + .1392 OH + .3219 $CH_2OO$ + .87 MGLYOX + .13 HCHO + .13 OH + .065 $HCOCOCH_2O_2$ + .065 CO + .065 $CH_3C(O)$ | 1.36E-15*EXP(-2112./temp) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44029 | TrGCN | MACR + $NO_3$ → MACO3 + $HNO_3$ | KNO3AL*2.0 | Rickard and Pascoe (2009) |
| G44030a | TrGC | MACO3 → $CH_3C(O)$ + HCHO + $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G44030b | TrGC | MACO3 → MACO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G44031a | TrGC | MACO3 + $HO_2$ → MACO2 + OH | KAPHO2*r_CO3_OH | Sander et al. (2019) |
| G44031b | TrGC | MACO3 + $HO_2$ → MACO3H | KAPHO2*r_CO3_OOH | Sander et al. (2019) |
| G44031c | TrGC | MACO3 + $HO_2$ → MACO2H + $O_3$ | KAPHO2*r_CO3_O3 | Sander et al. (2019) |
| G44032 | TrGCN | MACO3 + NO → MACO2 + $NO_2$ | 8.70E-12*EXP(290./temp) | Sander et al. (2019) |
| G44033 | TrGCN | MACO3 + $NO_2$ → MPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44034 | TrGCN | MACO3 + $NO_3$ → MACO2 + $NO_2$ | KRO2NO3*1.74 | Sander et al. (2019) |
| G44035 | TrGC | MACRO2 → .7 $CH_3COCH_2OH$ + .7 HCHO + .7 $HO_2$ + .3 MACROH | k1_RO2tORO2 | Rickard and Pascoe (2009)* |
| G44036a | TrGC | MACRO2 + $HO_2$ → MACRO + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Sander et al. (2019) |
| G44036b | TrGC | MACRO2 + $HO_2$ → MACROOH | k_RO2_HO2(temp,4)*r_COCH2O2_OOH | Sander et al. (2019) |
| G44037a | TrGCN | MACRO2 + NO → MACRO + $NO_2$ | KRO2NO*(1.-alpha_AN(6,3,1,0,0, temp,cair)) | Sander et al. (2019) |
| G44037b | TrGCN | MACRO2 + NO → MACRNO3 | KRO2NO*alpha_AN(6,3,1,0,0,temp, cair) | Sander et al. (2019) |
| G44038 | TrGCN | MACRO2 + $NO_3$ → MACRO + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44039a | TrGC | MACROOH + OH → MACRO2 | k_ROOHRO | Sander et al. (2019) |
| G44039b | TrGC | MACROOH + OH → CO + $CH_3COCH_2OH$ + OH | k_t*f_O*f_tCH2OH*f_alk | Sander et al. (2019) |
| G44039c | TrGC | MACROOH + OH → CO + MGLYOX + $HO_2$ | (k_s*f_sOH*f_pCH2OH + k_ROHRO) | Sander et al. (2019) |
| G44040 | TrGC | MACROH + OH → $CH_3COCH_2OH$ + CO + $HO_2$ | k_t*f_O*f_tCH2OH*f_alk | Sander et al. (2019) |
| G44041 | TrGC | MACRO → .885 $CH_3COCH_2OH$ + .885 CO + .115 MGLYOX + .115 HCHO + $HO_2$ | KDEC | Sander et al. (2019) |
| G44042 | TrGC | MACO2H + OH → $CH_3COCH_2OH$ + $HO_2$ + $CO_2$ | ((k_adt+k_adp)*a_CO2H+k_CO2H) | Sander et al. (2019) |
| G44043a | TrGC | MACO3H + OH → $CH_3COCH_2OH$ + $CO_2$ + OH | (k_adt+k_adp)*a_CO2H | Sander et al. (2019) |
| G44043b | TrGC | MACO3H + OH → MACO3 | k_ROOHRO | Sander et al. (2019) |
| G44044 | TrGC | LHMVKABO2 → .024 CO2H3CHO + .072 MGLYOX + .072 $HO_2$ + .072 HCHO + .5280 $CH_3C(O)$ + .5280 $HOCH_2CHO$ + .176 BIACETOH + .2 HO12CO3C4 | (.12*k1_RO2pORO2+.88*k1_RO2sORO2) | Sander et al. (2019) |
| G44045a | TrGC | LHMVKABO2 + $HO_2$ → OH + $HOCH_2CHO$ + $CH_3C(O)$ | k_RO2_HO2(temp,4)*.88*r_COCH2O2_ OH | Sander et al. (2019) |
| G44045b | TrGC | LHMVKABO2 + $HO_2$ → LHMVKABOOH | k_RO2_HO2(temp,4)*(.12+.88*r_ COCH2O2_OOH) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44046a | TrGCN | LHMVKABO2 + NO → .12 MGLYOX + .12 $HO_2$ + .88 $HOCH_2CHO$ + .88 $CH_3C(O)$ + .12 HCHO + $NO_2$ | `KRO2NO*(1.-(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)))` | Sander et al. (2019) |
| G44046b | TrGCN | LHMVKABO2 + NO → MVKNO3 | `KRO2NO*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair))` | Sander et al. (2019)* |
| G44047 | TrGCN | LHMVKABO2 + $NO_3$ → .12 MGLYOX + .12 $HO_2$ + .88 $HOCH_2CHO$ + .88 $CH_3C(O)$ + .12 HCHO + .12 $HO_2$ + $NO_2$ | `KRO2NO3` | Sander et al. (2019) |
| G44048a | TrGC | LHMVKABOOH + OH → LHMVKABO2 | `k_ROOHRO` | Sander et al. (2019) |
| G44048b | TrGC | LHMVKABOOH + OH → .12 CO2H3CHO + .88 BIACETOH + OH | `(.12*k_s*f_sOOH*f_pCH2OH+.88*k_t*f_tOOH*f_pCH2OH*f_CO)` | Sander et al. (2019) |
| G44049a | TrGC | CO2H3CHO + OH → CO2H3CO3 | `k_t*f_O*f_alk` | Sander et al. (2019) |
| G44049b | TrGC | CO2H3CHO + OH → $CH_3COCOCHO$ + $HO_2$ + $H_2O$ | `k_t*f_CO*f_tOH*f_CHO` | Sander et al. (2019) |
| G44050 | TrGCN | CO2H3CHO + $NO_3$ → CO2H3CO3 + $HNO_3$ | `KNO3AL*4.0` | Rickard and Pascoe (2009) |
| G44051 | TrGC | CO2H3CO3 → MGLYOX + $HO_2$ + $CO_2$ | `k1_RO2RCO3` | Sander et al. (2019) |
| G44052a | TrGC | CO2H3CO3 + $HO_2$ → OH + MGLYOX + $HO_2$ + $CO_2$ | `KAPHO2*r_CO3_OH` | Sander et al. (2019) |
| G44052b | TrGC | CO2H3CO3 + $HO_2$ → CO2H3CO2H + $O_3$ | `KAPHO2*r_CO3_O3` | Sander et al. (2019) |
| G44052c | TrGC | CO2H3CO3 + $HO_2$ → CO2H3CO3H | `KAPHO2*r_CO3_OOH` | Sander et al. (2019) |
| G44053 | TrGCN | CO2H3CO3 + NO → MGLYOX + $HO_2$ + $NO_2$ + $CO_2$ | `KAPNO` | Sander et al. (2019) |
| G44054 | TrGCN | CO2H3CO3 + $NO_3$ → MGLYOX + $HO_2$ + $NO_2$ + $CO_2$ | `KRO2NO3*1.74` | Sander et al. (2019) |
| G44055a | TrGC | CO2H3CO3H + OH → CO2H3CO3 | `k_ROOHRO` | Sander et al. (2019) |
| G44055b | TrGC | CO2H3CO3H + OH → $CH_3C(O)$ + CO + $CO_2$ + OH | `(k_t*f_CO2H*f_CO*f_tOH)` | Sander et al. (2019) |
| G44056 | TrGC | CO2H3CO2H + OH → CH3COCOCO2H + $HO_2$ | `k_t*f_CO2H*f_CO*f_tOH+k_CO2H` | Sander et al. (2019) |
| G44057a | TrGC | HO12CO3C4 + OH → BIACETOH + $HO_2$ | `k_t*f_tOH*f_alk*f_CO` | Sander et al. (2019) |
| G44057b | TrGC | HO12CO3C4 + OH → CO2H3CHO + $HO_2$ | `k_s*f_sOH*f_alk` | Sander et al. (2019) |
| G44058 | TrGC | MACO2 → .65 $CH_3$ + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + $CO_2$ | `KDEC` | Sander et al. (2019) |
| G44059 | TrGC | LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 $CH_3C(O)$ + OH | `k_hsd` | Sander et al. (2019) |
| G44060 | TrGC | MACRO2 → MGLYOX + HCHO + OH | `k_hsb` | Sander et al. (2019) |
| G44061a | TrGCN | MVKNO3 + OH → MGLYOX + $CO_2$ + $HO_2$ + $NO_2$ + $H_2O$ | `k_s*f_sOOH*f_CH2ONO2+k_ROHRO` | Sander et al. (2019)* |
| G44061b | TrGCN | MVKNO3 + OH → BIACETOH + $NO_2$ + $H_2O$ | `k_t*f_ONO2*f_CO*f_pCH2OH` | Sander et al. (2019)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44062a | TrGCN | MACRNO3 + OH → $CH_3COCH_2OH$ + $CO_2$ + $NO_2$ + $H_2O$ | k_t*f_O*f_CH2ONO2 | Sander et al. (2019)* |
| G44062b | TrGCN | MACRNO3 + OH → MGLYOX + CO + $NO_2$ + $H_2O$ | k_ROHRO+k_s*f_sOOH*f_CH2ONO2 | Sander et al. (2019)* |
| G44063 | TrGC | MACRO2 → $CH_3COCH_2OH$ + OH + CO | k_14hsal | Sander et al. (2019) |
| G44064 | TrGC | EZCH3CO2CHCHO → .9 $CH_3COCHCO$ + .1 $CH_3C(O)$ + .01 GLYOX + .18 CO + .09 $HO_2$ + OH | k_15hs24vynal | Sander et al. (2019) |
| G44065 | TrGC | EZCH3CO2CHCHO + $HO_2$→ $CH_3COOHCHCHO$ | k_RO2_HO2(temp,4) | Sander et al. (2019) |
| G44066 | TrGCN | EZCH3CO2CHCHO + NO → $CH_3COCHO_2CHO$ + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G44067 | TrGCN | EZCH3CO2CHCHO + $NO_3$→ $CH_3COCHO_2CHO$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44068 | TrGC | EZCH3CO2CHCHO → $CH_3COCHO_2CHO$ | k1_RO2sORO2 | Sander et al. (2019) |
| G44069 | TrGC | EZCHOCCH3CHO2 → $HCOCCH_3CO$ + OH | k_15hs24vynal | Sander et al. (2019) |
| G44070 | TrGCN | EZCHOCCH3CHO2 + NO → $HCOCO_2CH_3CHO$ + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G44071 | TrGC | EZCHOCCH3CHO2 + $HO_2$→ $HCOCCH_3CHOOH$ | k_RO2_HO2(temp,4) | Sander et al. (2019) |
| G44072 | TrGCN | EZCHOCCH3CHO2 + $NO_3$→ $HCOCO_2CH_3CHO$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44073 | TrGC | EZCHOCCH3CHO2 → $HCOCO_2CH_3CHO$ | k1_RO2pORO2 | Sander et al. (2019) |
| G44074 | TrGC | $CH_3COOHCHCHO$ → $CH_3COCHO_2CHO$ + OH | k_hydec | Sander et al. (2019) |
| G44075 | TrGC | $HCOCCH_3CHOOH$ → $HCOCO_2CH_3CHO$ + OH | k_hydec | Sander et al. (2019) |
| G44076 | TrGCN | $CH_3COCHO_2CHO$ + NO → $CH_3C(O)$ + GLYOX + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G44077 | TrGCN | $CH_3COCHO_2CHO$ + $NO_3$ → $CH_3C(O)$ + GLYOX + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44078 | TrGC | $CH_3COCHO_2CHO$ + $HO_2$ → $CH_3C(O)$ + GLYOX + OH | k_RO2_HO2(temp,4) | Sander et al. (2019)* |
| G44079 | TrGC | $CH_3COCHO_2CHO$ → $CH_3C(O)$ + GLYOX | k1_RO2sORO2 | Sander et al. (2019) |
| G44080 | TrGC | $HCOCO_2CH_3CHO$ → MGLYOX + CO + $HO_2$ | k1_RO2tORO2 | Sander et al. (2019) |
| G44081 | TrGCN | $HCOCO_2CH_3CHO$ + NO → MGLYOX + CO + $HO_2$ + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G44082 | TrGC | $HCOCO_2CH_3CHO$ + $HO_2$ → MGLYOX + CO + $HO_2$ + OH | k_RO2_HO2(temp,4) | Sander et al. (2019)* |
| G44083 | TrGCN | $HCOCO_2CH_3CHO$ + $NO_3$ → MGLYOX + CO + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44084 | TrGC | $HCOCCH_3CO$ + OH → CO + MGLYOX + $HO_2$ | 1E-10*a_CHO | Hatakeyama et al. (1985), Sander et al. (2019) |
| G44085 | TrGC | $CH_3COCHCO$ + OH → CO + MGLYOX + $HO_2$ | 7.6E-11*a_COCH3 | Hatakeyama et al. (1985), Sander et al. (2019)* |
| G44086 | TrGCN | LMEKNO3 + OH → .62 MGLYOX + .62 HCHO + .62 $HO_2$ + .62 $NO_2$ + .38 $CH_3C(O)$ + .38 $NO_3CH2CHO$ | .62*(k_p*(f_CO+f_CH2ONO2)) +.38*(k_s*f_CH2ONO2*f_CO) | Sander et al. (2019)* |
| G44087 | TrGC | MEPROPENE + OH → IBUTOLBO2 | 9.4E-12*EXP(505./temp) | Atkinson et al. (2006) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44088a | TrGC | MEPROPENE + $O_3$ → $CH_3COCH_3$ + $CH_2OO^*$ | 2.7E-15*EXP(-1630./temp)*0.33 | Atkinson et al. (2006), Sander et al. (2019) |
| G44088b | TrGC | MEPROPENE + $O_3$ → $CH_3COCH_2O_2$ + OH + HCHO | 2.7E-15*EXP(-1630./temp)*0.67 | Atkinson et al. (2006), Sander et al. (2019) |
| G44089 | TrGCN | MEPROPENE + $NO_3$ → $CH_3COCH_3$ + HCHO + $NO_2$ | 3.4E-13 | Atkinson et al. (2006), Sander et al. (2019)* |
| G44090 | TrGC | IBUTOLBO2 → $CH_3COCH_3$ + HCHO + $HO_2$ | k1_RO2tORO2 | Sander et al. (2019) |
| G44091a | TrGC | IBUTOLBO2 + $HO_2$ → IBUTOLBOOH | k_RO2_HO2(temp,4)*r_COCH2O2_OOH | Sander et al. (2019) |
| G44091b | TrGC | IBUTOLBO2 + $HO_2$ → $CH_3COCH_3$ + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Sander et al. (2019) |
| G44092a | TrGCN | IBUTOLBO2 + NO → $CH_3COCH_3$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(5,3,0,0,0, temp,cair)) | Sander et al. (2019) |
| G44092b | TrGCN | IBUTOLBO2 + NO → IBUTOLBNO3 | KRO2NO*alpha_AN(5,3,0,0,0,temp, cair) | Sander et al. (2019) |
| G44093 | TrGCN | IBUTOLBO2 + $NO_3$ → $CH_3COCH_3$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44094a | TrGC | IBUTOLBOOH + OH → IBUTOLBO2 | k_ROOHRO | Sander et al. (2019) |
| G44094b | TrGC | IBUTOLBOOH + OH → $CH_3COCH_3$ + HCHO + $HO_2$ | k_s*f_sOOH*f_pCH2OH | Sander et al. (2019) |
| G44095 | TrGCN | IBUTOLBNO3 + OH → $CH_3COCH_3$ + HCHO + $HO_2$ + $NO_2$ | 3.*k_p | Sander et al. (2019) |
| G44096 | TrGC | BUT1ENE + OH → LBUT1ENO2 | 6.6E-12*EXP(465./temp) | Atkinson et al. (2006)* |
| G44097a | TrGC | BUT1ENE + $O_3$ → HCHO + .5 $C_2H_5CHO$ + .5 $H_2O_2$ + .5 $CH_3CHO$ + .5 CO + .5 $HO_2$ | 3.35E-15*EXP(-1745./temp)*.57 | Atkinson et al. (2006), Sander et al. (2019)* |
| G44097b | TrGC | BUT1ENE + $O_3$ → $C_2H_5CHO$ + $CH_2OO^*$ | 3.35E-15*EXP(-1745./temp)*.43 | Atkinson et al. (2006), Sander et al. (2019)* |
| G44098 | TrGCN | BUT1ENE + $NO_3$ → $C_2H_5CHO$ + HCHO + $NO_2$ | 3.2E-13*EXP(-950./temp) | Atkinson et al. (2006), Sander et al. (2019)* |
| G44099 | TrGC | LBUT1ENO2 → $C_2H_5CHO$ + HCHO + $HO_2$ | k1_RO2sORO2 | Sander et al. (2019) |
| G44100a | TrGC | LBUT1ENO2 + $HO_2$ → LBUT1ENOOH | k_RO2_HO2(temp,4)*r_COCH2O2_OOH | Sander et al. (2019) |
| G44100b | TrGC | LBUT1ENO2 + $HO_2$ → $C_2H_5CHO$ + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Sander et al. (2019) |
| G44101a | TrGCN | LBUT1ENO2 + NO → $C_2H_5CHO$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair)) | Sander et al. (2019) |
| G44101b | TrGCN | LBUT1ENO2 + NO → LBUT1ENNO3 | KRO2NO*alpha_AN(5,2,0,0,0,temp, cair) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44102 | TrGCN | LBUT1ENO2 + $NO_3$ → $C_2H_5CHO$ + HCHO + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44103a | TrGC | LBUT1ENOOH + OH → LBUT1ENO2 | k_ROOHRO | Sander et al. (2019) |
| G44103b | TrGC | LBUT1ENOOH + OH → $C_2H_5CO_3$ + HCHO + $HO_2$ | k_t*f_tOOH*f_pCH2OH | Sander et al. (2019)* |
| G44104 | TrGCN | LBUT1ENNO3 + OH → $C_2H_5CHO$ + CO + $HO_2$ + $NO_2$ | k_s*f_sOH*f_CH2ONO2 | Sander et al. (2019)* |
| G44105 | TrGC | CBUT2ENE + OH → BUT2OLO2 | 1.1E-11*EXP(485./temp) | Atkinson et al. (2006) |
| G44106 | TrGC | CBUT2ENE + $O_3$ → $CH_3CHO$ + .16 CH3CHOHOOH + .50 OH + .50 $HCOCH_2O_2$ + .05 CH2CO + .09 $CH_3OH$ + .09 CO + .2 $CH_4$ + .2 $CO_2$ | 3.2E-15*EXP(-965./temp) | Atkinson et al. (2006), Sander et al. (2019)* |
| G44107 | TrGCN | CBUT2ENE + $NO_3$ → 2 $CH_3CHO$ + $NO_2$ | 3.5E-13 | Atkinson et al. (2006), Sander et al. (2019)* |
| G44108 | TrGC | TBUT2ENE + OH → BUT2OLO2 | 1.0E-11*EXP(553./temp) | Atkinson et al. (2006) |
| G44109 | TrGC | TBUT2ENE + $O_3$ → $CH_3CHO$ + .16 CH3CHOHOOH + .50 OH + .50 $HCOCH_2O_2$ + .05 CH2CO + .09 $CH_3OH$ + .09 CO + .2 $CH_4$ + .2 $CO_2$ | 6.6E-15*EXP(-1060./temp) | Atkinson et al. (2006), Sander et al. (2019) |
| G44110 | TrGCN | TBUT2ENE + $NO_3$ → 2 $CH_3CHO$ + $NO_2$ | 1.78E-12*EXP(-530./temp) +1.28E-14*EXP(570./temp) | Atkinson et al. (2006), Sander et al. (2019)* |
| G44111 | TrGC | BUT2OLO2 → $C_2H_5CHO$ + HCHO + $HO_2$ | k1_RO2sORO2 | Sander et al. (2019) |
| G44112a | TrGC | BUT2OLO2 + $HO_2$ → BUT2OLOOH | k_RO2_HO2(temp,4)*r_COCH2O2_OOH | Sander et al. (2019) |
| G44112b | TrGC | BUT2OLO2 + $HO_2$ → 2 $CH_3CHO$ + $HO_2$ + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Sander et al. (2019) |
| G44113a | TrGCN | BUT2OLO2 + NO → 2 $CH_3CHO$ + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair)) | Sander et al. (2019) |
| G44113b | TrGCN | BUT2OLO2 + NO → BUT2OLNO3 | KRO2NO*alpha_AN(5,2,0,0,0,temp, cair) | Sander et al. (2019) |
| G44114 | TrGCN | BUT2OLO2 + $NO_3$ → 2 $CH_3CHO$ + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G44115a | TrGC | BUT2OLOOH + OH → BUT2OLO2 | k_ROOHRO | Sander et al. (2019) |
| G44115b | TrGC | BUT2OLOOH + OH → LMEKOOH + $HO_2$ | k_t*f_tOH*f_pCH2OH | Sander et al. (2019) |
| G44115c | TrGC | BUT2OLOOH + OH → BUT2OLO + OH | k_t*f_tOOH*f_pCH2OH | Sander et al. (2019) |
| G44116 | TrGCN | BUT2OLNO3 + OH → LMEKNO3 + $HO_2$ | k_t*f_tOH*f_CH2ONO2 | Sander et al. (2019) |
| G44117 | TrGC | BUT2OLO + OH → BIACET + $HO_2$ | k_t*f_tOH*f_CO | Sander et al. (2019) |
| G44118 | TrGC | IPRCHO + OH → IPRCO3 + $H_2O$ | 6.8E-12*EXP(410./temp) | Atkinson et al. (2006) |
| G44119 | TrGCN | IPRCHO + $NO_3$ → IPRCO3 + $HNO_3$ | 1.67E-12*EXP(-1460./temp) | Atkinson et al. (2006) |
| G44120 | TrGC | IPRCO3 → $iC_3H_7O_2$ + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G44121a | TrGC | IPRCO3 + $HO_2$ → PERIBUACID | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44121b | TrGC | IPRCO3 + $HO_2$ → $iC_3H_7O_2$ + $CO_2$ + OH | `KAPHO2*(1.-r_CO3_OOH)` | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44122 | TrGCN | IPRCO3 + $NO_2$ → PIPN | `k_CH3CO3_NO2` | Rickard and Pascoe (2009) |
| G44123 | TrGCN | IPRCO3 + NO → $iC_3H_7O_2$ + $CO_2$ + $NO_2$ | `KAPNO` | Rickard and Pascoe (2009) |
| G44124a | TrGC | PERIBUACID + OH → IPRCO3 + $H_2O$ | `k_ROOHRO` | Rickard and Pascoe (2009) |
| G44124b | TrGC | PERIBUACID + OH → $CH_3COCH_3$ + $H_2O$ + $CO_2$ | `k_s*f_CO2H` | Sander et al. (2019)* |
| G44125 | TrGCN | PIPN → IPRCO3 + $NO_2$ | `k_PAN_M` | Rickard and Pascoe (2009) |
| G44126 | TrGCN | PIPN + OH → $CH_3COCH_3$ + $CO_2$ + $NO_2$ | `k_s*f_cpan` | Sander et al. (2019)* |
| G44127 | TrGC | MPROPENOL + OH → HCOOH + OH + $CH_3COCH_3$ | `k_CH2CHOH_OH_HCOOH` | Sander et al. (2019), So et al. (2014)* |
| G44128 | TrGC | MPROPENOL + HCOOH → IPRCHO + HCOOH | `k_CH2CHOH_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44129 | TrGC | IPRCHO + HCOOH → MPROPENOL + HCOOH | `k_ALD_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44130 | TrGC | BUTENOL + OH → HCOOH + OH + $C_2H_5CHO$ | `k_CH2CHOH_OH_HCOOH` | Sander et al. (2019), So et al. (2014)* |
| G44131 | TrGC | BUTENOL + HCOOH → $C_3H_7CHO$ + HCOOH | `k_CH2CHOH_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44132 | TrGC | $C_3H_7CHO$ + HCOOH → BUTENOL + HCOOH | `k_ALD_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44133 | TrGC | HVMK + OH → HCOOH + OH + MGLYOX | `8.8E-11` | Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)* |
| G44134 | TrGC | HVMK + HCOOH → CO2C3CHO + HCOOH | `k_CH2CHOH_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44135 | TrGC | CO2C3CHO + HCOOH → HVMK + HCOOH | `k_ALD_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44136 | TrGC | HMAC + OH → HCOOH + OH + MGLYOX | `8.8E-11` | Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)* |
| G44137 | TrGC | HMAC + HCOOH → IBUTDIAL + HCOOH | `k_CH2CHOH_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44138 | TrGC | IBUTDIAL + HCOOH → HMAC + HCOOH | `k_ALD_HCOOH` | Sander et al. (2019), da Silva (2010)* |
| G44139 | TrGC | CO2C3CHO + OH → $CH_3COCH_2O_2$ + $CO_2$ + $H_2O$ | `k_t*f_O*f_alk+k_s*f_CHO*f_CO` | Sander et al. (2019)* |
| G44140 | TrGCN | CO2C3CHO + $NO_3$ → $CH_3COCH_2O_2$ + $CO_2$ + $HNO_3$ | `KNO3AL*4.0` | Sander et al. (2019)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44141 | TrGC | IBUTDIAL + OH $\rightarrow$ $CH_3CHO$ + CO + $HO_2$ + $CO_2$ + $H_2O$ | 2.*k_t*f_O*f_alk+k_t*f_CHO*f_CHO | Sander et al. (2019)* |
| G44142 | TrGCN | IBUTDIAL + $NO_3$ $\rightarrow$ $CH_3CHO$ + CO + $HO_2$ + $CO_2$ + $HNO_3$ | 2.*KNO3AL*4.0 | Sander et al. (2019)* |
| G44200 | TrGTerC | $CH_3COCOCH_2O_2$ $\rightarrow$ $CH_3C(O)$ + HCHO + CO | k1_RO2pORO2 | Rickard and Pascoe (2009) |
| G44201 | TrGTerC | $CH_3COCOCH_2O_2$ + $HO_2$ $\rightarrow$ $CH_3COCOCH_2OOH$ | k_RO2_HO2(temp,4) | Rickard and Pascoe (2009) |
| G44202 | TrGTerCN | $CH_3COCOCH_2O_2$ + NO $\rightarrow$ $CH_3C(O)$ + HCHO + CO + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44203a | TrGTerC | $CH_3COCOCH_2OOH$ + OH $\rightarrow$ $CH_3COCOCHO$ + OH | k_s*f_CO*f_sOOH | Rickard and Pascoe (2009)* |
| G44203b | TrGTerC | $CH_3COCOCH_2OOH$ + OH $\rightarrow$ $CH_3COCOCH_2O_2$ | k_ROOHRO | Rickard and Pascoe (2009) |
| G44204 | TrGTerC | C44O2 + $HO_2$ $\rightarrow$ C44OOH | k_RO2_HO2(temp,4) | Rickard and Pascoe (2009) |
| G44205 | TrGTerCN | C44O2 + NO $\rightarrow$ HCOCH2CHO + $CO_2$ + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44206 | TrGTerC | C44O2 $\rightarrow$ HCOCH2CHO + $CO_2$ + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G44207 | TrGTerC | C44OOH + OH $\rightarrow$ C44O2 | 7.46E-11 | Rickard and Pascoe (2009) |
| G44208 | TrGTerC | CHOC3COO2 $\rightarrow$ HCOCH2CO3 + HCHO | k1_RO2pORO2 | Rickard and Pascoe (2009) |
| G44209 | TrGTerC | CHOC3COO2 + $HO_2$ $\rightarrow$ C413COOOH | k_RO2_HO2(temp,4) | Rickard and Pascoe (2009) |
| G44210 | TrGTerCN | CHOC3COO2 + NO $\rightarrow$ HCOCH2CO3 + HCHO + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44211 | TrGTerC | C413COOOH + OH $\rightarrow$ CHOC3COO2 | 8.33E-11 | Rickard and Pascoe (2009) |
| G44212 | TrGTerC | C4CODIAL + OH $\rightarrow$ C312COCO3 | 3.39E-11 | Rickard and Pascoe (2009) |
| G44213 | TrGTerCN | C4CODIAL + $NO_3$ $\rightarrow$ C312COCO3 + $HNO_3$ | 2.*KNO3AL*4.0 | Rickard and Pascoe (2009) |
| G44214 | TrGTerC | C312COCO3 $\rightarrow$ $HCOCOCH_2O_2$ + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G44215a | TrGTerC | C312COCO3 + $HO_2$ $\rightarrow$ C312COCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G44215b | TrGTerC | C312COCO3 + $HO_2$ $\rightarrow$ $HCOCOCH_2O_2$ + $CO_2$ + OH | KAPHO2*(1.-r_CO3_OOH) | Rickard and Pascoe (2009) |
| G44216 | TrGTerCN | C312COCO3 + $NO_2$ $\rightarrow$ C312COPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44217 | TrGTerCN | C312COCO3 + NO $\rightarrow$ $HCOCOCH_2O_2$ + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G44218 | TrGTerC | C312COCO3H + OH $\rightarrow$ C312COCO3 | 1.63E-11 | Rickard and Pascoe (2009) |
| G44219 | TrGTerCN | C312COPAN $\rightarrow$ C312COCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G44220 | TrGTerCN | C312COPAN + OH $\rightarrow$ HCOCOCHO + CO + $NO_2$ | 1.27E-11 | Rickard and Pascoe (2009) |
| G44221 | TrGTerC | $CH_3COCOCHO$ + OH $\rightarrow$ $CH_3C(O)$ + 2 CO | 8.4E-13*EXP(830./temp) | Sander et al. (2019)* |
| G44222 | TrGTerCN | $CH_3COCOCHO$ + $NO_3$ $\rightarrow$ $CH_3C(O)$ + 2 CO + $HNO_3$ | KNO3AL*4.0 | Rickard and Pascoe (2009) |
| G44223 | TrGTerC | IBUTALOH + OH $\rightarrow$ IPRHOCO3 | 1.4E-11 | Rickard and Pascoe (2009) |
| G44224a | TrGTerC | IPRHOCO3 + $HO_2$ $\rightarrow$ $CH_3COCH_3$ + $CO_2$ + $HO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44224b | TrGTerC | IPRHOCO3 + $HO_2$ $\rightarrow$ IPRHOCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009), Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44224c | TrGTerC | IPRHOCO3 + $HO_2$ → IPRHOCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44225 | TrGTerCN | IPRHOCO3 + NO → $CH_3COCH_3$ + $CO_2$ + $HO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G44226 | TrGTerCN | IPRHOCO3 + $NO_2$ → C4PAN5 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44227 | TrGTerCN | IPRHOCO3 + $NO_3$ → $CH_3COCH_3$ + $CO_2$ + $HO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G44228a | TrGTerC | IPRHOCO3 → $CH_3COCH_3$ + $CO_2$ + $HO_2$ | k1_RO2RCO3*0.7 | Rickard and Pascoe (2009) |
| G44228b | TrGTerC | IPRHOCO3 → IPRHOCO2H | k1_RO2RCO3*0.3 | Rickard and Pascoe (2009) |
| G44229 | TrGTerC | IPRHOCO2H + OH → $CH_3COCH_3$ + $CO_2$ + $HO_2$ + $H_2O$ | 1.72E-12 | Rickard and Pascoe (2009) |
| G44230 | TrGTerC | OH + IPRHOCO3H → IPRHOCO3 | 4.80E-12 | Rickard and Pascoe (2009) |
| G44231 | TrGTerCN | C4PAN5 → IPRHOCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G44232 | TrGTerCN | C4PAN5 + OH → $CH_3COCH_3$ + CO + $NO_2$ | 4.75E-13 | Rickard and Pascoe (2009) |
| G44233a | TrGTerC | MBOOO → IPRHOCO2H | 1.60E-17*C(ind_H2O)*(0.08+0.15) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44233b | TrGTerC | MBOOO → IBUTALOH + $H_2O_2$ | 1.60E-17*C(ind_H2O)*0.77 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44234 | TrGTerC | MBOOO + CO → IBUTALOH + $CO_2$ | 1.20E-15 | Rickard and Pascoe (2009) |
| G44235 | TrGTerCN | MBOOO + NO → IBUTALOH + $NO_2$ | 1.00E-14 | Rickard and Pascoe (2009) |
| G44236 | TrGTerCN | MBOOO + $NO_2$ → IBUTALOH + $NO_3$ | 1.00E-15 | Rickard and Pascoe (2009) |
| G44400 | TrGAroC | MALANHY + OH → MALANHYO2 | 1.4E-12 | Rickard and Pascoe (2009) |
| G44401a | TrGAroC | MALDIALOOH + OH → HOCOC4DIAL + OH | 1.22E-10 | Rickard and Pascoe (2009) |
| G44401b | TrGAroC | MALDIALOOH + OH → MALDIALO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G44402 | TrGAroCN | NC4DCO2H + OH → MALANHY + $NO_2$ | k_ROOHRO | Rickard and Pascoe (2009)* |
| G44403 | TrGAroC | CO14O3CO2H + OH → $HCOCH_2O_2$ + 2 $CO_2$ | 2.19E-11 | Rickard and Pascoe (2009) |
| G44404 | TrGAroC | BZFUOOH + OH → BZFUO2 | 3.68E-11 | Rickard and Pascoe (2009) |
| G44405 | TrGAroC | HOCOC4DIAL + OH → CO2C4DIAL + $HO_2$ | 3.67E-11 | Rickard and Pascoe (2009) |
| G44406a | TrGAroC | MALDIALCO3 + $HO_2$ → MALDALCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G44406b | TrGAroC | MALDIALCO3 + $HO_2$ → MALDALCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G44406c | TrGAroC | MALDIALCO3 + $HO_2$ → .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009)* |
| G44407 | TrGAroCN | MALDIALCO3 + NO → .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G44408 | TrGAroCN | MALDIALCO3 + $NO_2$ → MALDIALPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44409 | TrGAroCN | MALDIALCO3 + $NO_3$ → .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44410 | TrGAroC | MALDIALCO3 → .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G44411 | TrGAroCN | BZFUONE + $NO_3$ → NBZFUO2 | 3.00E-13 | Rickard and Pascoe (2009) |
| G44412 | TrGAroC | BZFUONE + $O_3$ → .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 $H_2O_2$ + .5 CO + .5 $CO_2$ + .5 $HCOCH_2O_2$ + .5 OH | 2.20E-19 | see note* |
| G44413 | TrGAroC | BZFUONE + OH → BZFUO2 | 4.45E-11 | Rickard and Pascoe (2009) |
| G44414 | TrGAroCN | NBZFUOOH + OH → NBZFUO2 | 6.18E-12 | Rickard and Pascoe (2009) |
| G44415 | TrGAroC | MALDALCO3H + OH → MALDIALCO3 | 4.00E-11 | Rickard and Pascoe (2009) |
| G44416 | TrGAroC | EPXDLCO2H + OH → C3DIALO2 + $CO_2$ | 2.31E-11 | Rickard and Pascoe (2009) |
| G44417a | TrGAroC | EPXDLCO3 + $HO_2$ → C3DIALO2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G44417b | TrGAroC | EPXDLCO3 + $HO_2$ → EPXDLCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G44417c | TrGAroC | EPXDLCO3 + $HO_2$ → EPXDLCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G44418 | TrGAroCN | EPXDLCO3 + NO → C3DIALO2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G44419 | TrGAroCN | EPXDLCO3 + $NO_2$ → EPXDLPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44420 | TrGAroCN | EPXDLCO3 + $NO_3$ → C3DIALO2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G44421 | TrGAroC | EPXDLCO3 → C3DIALO2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G44422 | TrGAroC | MALNHYOHCO + OH → CO + CO + CO + $CO_2$ + $HO_2$ | 5.68E-12 | Rickard and Pascoe (2009) |
| G44423 | TrGAroCN | MALDIAL + $NO_3$ → MALDIALCO3 + $HNO_3$ | 2.*KNO3AL*2.0 | Rickard and Pascoe (2009) |
| G44424 | TrGAroC | MALDIAL + $O_3$ → 1.0675 GLYOX + .125 HCHO + .1125 $HCOCO_2H$ + .0675 $H_2O_2$ + .82 $HO_2$ + .57 OH + 1.265 CO + .25 $CO_2$ | 2.00E-18 | Rickard and Pascoe (2009)* |
| G44425 | TrGAroC | MALDIAL + OH → .83 MALDIALCO3 + .17 MALDIALO2 | 5.20E-11 | Rickard and Pascoe (2009)* |
| G44426 | TrGAroC | MALANHYOOH + OH → MALNHYOHCO + OH | 4.66E-11 | Rickard and Pascoe (2009) |
| G44427 | TrGAroCN | MALDIALPAN + OH → GLYOX + CO + CO + $NO_2$ | 3.70E-11 | Rickard and Pascoe (2009) |
| G44428 | TrGAroCN | MALDIALPAN → MALDIALCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G44429a | TrGAroC | MALANHYO2 + $HO_2$ → MALANHYOOH | k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44429b | TrGAroC | MALANHYO2 + $HO_2$ → HCOCOHCO3 + $CO_2$ + OH | k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44430 | TrGAroCN | MALANHYO2 + NO → HCOCOHCO3 + $CO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44431 | TrGAroCN | MALANHYO2 + $NO_3$ → HCOCOHCO3 + $CO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G44432 | TrGAroC | MALANHYO2 → HCOCOHCO3 + $CO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G44433 | TrGAroC | EPXDLCO3H + OH → EPXDLCO3 | 2.62E-11 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44434 | TrGAroC | CO2C4DIAL + OH → CO + CO + CO + CO + $HO_2$ | 2.45E-11 | Rickard and Pascoe (2009) |
| G44435a | TrGAroCN | NBZFUO2 + $HO_2$ → NBZFUOOH | k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44435b | TrGAroCN | NBZFUO2 + $HO_2$ → .5 CO14O3CHO + .5 $NO_2$ + .5 NBZFUONE + .5 $HO_2$ + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44436 | TrGAroCN | NBZFUO2 + NO → .5 CO14O3CHO + .5 $NO_2$ + .5 NBZFUONE + .5 $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44437 | TrGAroCN | NBZFUO2 + $NO_3$ → .5 CO14O3CHO + .5 $NO_2$ + .5 NBZFUONE + .5 $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G44438 | TrGAroCN | NBZFUO2 → .5 CO14O3CHO + .5 $NO_2$ + .5 NBZFUONE + .5 $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G44439 | TrGAroC | MALDALCO2H + OH → .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ | 3.70E-11 | Rickard and Pascoe (2009)* |
| G44440 | TrGAroCN | EPXC4DIAL + $NO_3$ → EPXDLCO3 + $HNO_3$ | 2.*KNO3AL*4.0 | Rickard and Pascoe (2009) |
| G44441 | TrGAroC | EPXC4DIAL + OH → EPXDLCO3 | 4.32E-11 | Rickard and Pascoe (2009) |
| G44442a | TrGAroC | MECOACETO2 + $HO_2$ → MECOACEOOH | k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44442b | TrGAroC | MECOACETO2 + $HO_2$ → $CH_3C(O)OO$ + HCHO + $CO_2$ + OH | k_RO2_HO2(temp,4)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44443 | TrGAroCN | MECOACETO2 + NO → $CH_3C(O)OO$ + HCHO + $CO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44444 | TrGAroCN | MECOACETO2 + $NO_3$ → $CH_3C(O)OO$ + HCHO + $CO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G44445 | TrGAroC | MECOACETO2 → $CH_3C(O)OO$ + HCHO + $CO_2$ | k1_RO2pORO2 | Rickard and Pascoe (2009)* |
| G44446 | TrGAroCN | CO14O3CHO + $NO_3$ → CO + $HCOCH_2O_2$ + $CO_2$ + $HNO_3$ | KNO3AL*8.0 | Rickard and Pascoe (2009) |
| G44447 | TrGAroC | CO14O3CHO + OH → CO + $HCOCH_2O_2$ + $CO_2$ | 3.44E-11 | Rickard and Pascoe (2009) |
| G44448 | TrGAroCN | NBZFUONE + OH → BZFUCO + $NO_2$ | 1.16E-12 | Rickard and Pascoe (2009) |
| G44449a | TrGAroC | BZFUO2 + $HO_2$ → BZFUOOH | k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44449b | TrGAroC | BZFUO2 + $HO_2$ → CO14O3CHO + $HO_2$ + OH | k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G44450 | TrGAroCN | BZFUO2 + NO → CO14O3CHO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44451 | TrGAroCN | BZFUO2 + $NO_3$ → CO14O3CHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G44452 | TrGAroC | BZFUO2 → CO14O3CHO + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G44453 | TrGAroC | BZFUCO + OH → CO14O3CHO + $HO_2$ | 1.78E-11 | Rickard and Pascoe (2009) |
| G44456a | TrGAroC | MALDIALO2 + $HO_2$ → MALDIALOOH | k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G44456b | TrGAroC | MALDIALO2 + $HO_2$ → GLYOX + GLYOX + $HO_2$ + OH | k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G44457 | TrGAroCN | MALDIALO2 + NO → GLYOX + GLYOX + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G44458 | TrGAroCN | MALDIALO2 + $NO_3$ → GLYOX + GLYOX + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G44459 | TrGAroC | MALDIALO2 → GLYOX + GLYOX + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G44460 | TrGAroCN | EPXDLPAN + OH → HCOCOCHO + CO + $NO_2$ | 2.29E-11 | Rickard and Pascoe (2009) |
| G44461 | TrGAroCN | EPXDLPAN → EPXDLCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009)* |
| G44462 | TrGAroC | MECOACEOOH + OH → MECOACETO2 | 3.59E-12 | Rickard and Pascoe (2009) |
| G45000 | TrGC | $C_5H_8$ + $O_3$ → .3508 MACR + .01518 MACO2H + .2440 MVK + .7085 HCHO + .11 $CH_2OO$ + .1275 $C_3H_6$ + .1575 $CH_3C(O)$ + .0510 $CH_3$ + .2625 $HO_2$ + .27 OH + .09482 $H_2O_2$ + .255 $CO_2$ + .522 CO + .07182 HCHO + .03618 $HCOCH_2O_2$ + .01782 CO + 0.05408 LCARBON | 1.03E-14*EXP(-1995./temp) | Atkinson et al. (2006), Sander et al. (2019) |
| G45001 | TrGC | $C_5H_8$ + OH → .63 LISOPAB + .30 LISOPCD + .07 LISOPEFO2 | 2.7E-11*EXP(390./temp) | Atkinson et al. (2006), Sander et al. (2019) |
| G45002 | TrGCN | $C_5H_8$ + $NO_3$ → NISOPO2 | 3.0E-12*EXP(-450./temp) | Atkinson et al. (2006) |
| G45003a | TrGC | LISOPAB + $O_2$ → LISOPACO2 | 5.530E-13 | Sander et al. (2019) |
| G45003b | TrGC | LISOPAB + $O_2$ → ISOPBO2 | 3.E-12 | Sander et al. (2019) |
| G45004a | TrGC | LISOPCD + $O_2$ → LDISOPACO2 | 6.780E-13 | Sander et al. (2019) |
| G45004b | TrGC | LISOPCD + $O_2$ → ISOPDO2 | 3.E-12 | Sander et al. (2019) |
| G45005 | TrGC | LISOPACO2 → LISOPAB + $O_2$ | 3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4 | Sander et al. (2019) |
| G45006 | TrGC | ISOPBO2 → LISOPAB + $O_2$ | 3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp) | Sander et al. (2019) |
| G45007 | TrGC | LDISOPACO2 → LISOPCD + $O_2$ | 5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58 | Sander et al. (2019) |
| G45008 | TrGC | ISOPDO2 → LISOPCD + $O_2$ | 5.0E14*exp(-10120./temp)+8.25E14*exp(-10220./temp) | Sander et al. (2019) |
| G45009a | TrGC | LISOPACO2 → C1ODC2O2C4OOH | k_16hsz14 * 2./3.*(1.-f_HPAL) | Sander et al. (2019) |
| G45009b | TrGC | LISOPACO2 → LZCODC23DBCOOH + $HO_2$ | k_16hsz14 * (2./3.*f_HPAL + 1./3.) | Sander et al. (2019) |
| G45010a | TrGC | LDISOPACO2 → C1OOHC3O2C4OD | k_16hsz41 * 2./3.*(1.-f_HPAL) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45010b | TrGC | LDISOPACO2 → LZCODC23DBCOOH + $HO_2$ | k_16hsz41 * (2./3.*f_HPAL + 1./3.) | Sander et al. (2019) |
| G45011 | TrGC | LISOPACO2 → .9 LISOPACO + .1 ISOPAOH | k1_RO2LISOPACO2 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45012 | TrGC | LISOPACO2 + $HO_2$ → LISOPACOOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009) |
| G45013a | TrGCN | LISOPACO2 + NO → LISOPACO + $NO_2$ | KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair)) | Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019) |
| G45013b | TrGCN | LISOPACO2 + NO → LISOPACNO3 | KRO2NO*alpha_AN(6,1,0,0,0,temp, cair) | Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019) |
| G45014 | TrGCN | LISOPACO2 + $NO_3$ → LISOPACO + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45015 | TrGC | LDISOPACO2 → .9 LISOPACO + .1 ISOPAOH | k1_RO2LISOPACO2 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45016 | TrGC | LDISOPACO2 + $HO_2$ → LISOPACOOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009) |
| G45017a | TrGCN | LDISOPACO2 + NO → LISOPACO + $NO_2$ | KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair)) | Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019) |
| G45017b | TrGCN | LDISOPACO2 + NO → LISOPACNO3 | KRO2NO*alpha_AN(6,1,0,0,0,temp, cair) | Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019) |
| G45018 | TrGCN | LDISOPACO2 + $NO_3$ → LISOPACO + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45019a | TrGC | LISOPACOOH + OH → LISOPACO2 | k_ROOHRO | Sander et al. (2019) |
| G45019b | TrGC | LISOPACOOH + OH → LZCODC23DBCOOH + $HO_2$ | k_s*f_allyl*f_sOH | Sander et al. (2019) |
| G45019c | TrGC | LISOPACOOH + OH → LHC4ACCHO + OH | (k_s*f_sOOH*f_allyl+ k_ROHRO) | Sander et al. (2019) |
| G45019d | TrGC | LISOPACOOH + OH → LIEPOX + OH | (k_adt+k_ads)*a_CH2OH*a_CH2OOH | Sander et al. (2019)* |
| G45020 | TrGC | ISOPAOH + OH → LHC4ACCHO + $HO_2$ | (k_adt+k_ads)*a_CH2OH*a_CH2OH+k_ s*f_sOH*f_allyl+k_ROHRO | Sander et al. (2019) |
| G45021 | TrGCN | LISOPACNO3 + OH → LISOPACNO3O2 | (k_adt+k_ads)*a_CH2ONO2*a_CH2OH | Sander et al. (2019)* |
| G45022 | TrGC | ISOPBO2 → .8 MVK + .8 HCHO + .8 $HO_2$ + .2 ISOPBOH | k1_RO2ISOPBO2 | Rickard and Pascoe (2009) |
| G45023a | TrGC | ISOPBO2 + $HO_2$ → ISOPBOOH | k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH) | Sander et al. (2019) |
| G45023b | TrGC | ISOPBO2 + $HO_2$ → MVK + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH | Sander et al. (2019) |
| G45024a | TrGCN | ISOPBO2 + NO → MVK + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(6,3,0,0,0, temp,cair)) | Lockwood et al. (2010), Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45024b | TrGCN | ISOPBO2 + NO → ISOPBNO3 | KRO2NO*alpha_AN(6,3,0,0,0,temp, cair) | Lockwood et al. (2010), Sander et al. (2019) |
| G45025 | TrGCN | ISOPBO2 + $NO_3$ → MVK + .75 HCHO + .75 $HO_2$ + .25 $CH_3$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45026a | TrGC | ISOPBOOH + OH → LIEPOX + OH | (k_ads+k_adp)*a_CH2OOH | Paulot et al. (2009b), Sander et al. (2019) |
| G45026b | TrGC | ISOPBOOH + OH → ISOPBO2 | k_ROOHRO | Sander et al. (2019) |
| G45026c | TrGC | ISOPBOOH + OH → MGLYOX + $HOCH_2CHO$ | k_ROHRO+k_s*f_alk*f_sOH | Sander et al. (2019) |
| G45027 | TrGC | ISOPBOOH + $O_3$ → .1368 MACROOH + .1368 $H_2O_2$ + .2280 $HO_2$ + .4332 $CH_3COCH_2OH$ + .2280 $CO_2$ + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 $HO_2$ + .06880 OH + .2709 CO + .1591 $CH_2OO$ | 1.E-17 | Sander et al. (2019) |
| G45028 | TrGC | ISOPBOH + OH → MVK + .75 HCHO + .75 $HO_2$ + .25 $CH_3$ | k_s*f_alk*f_sOH+(k_adp+k_ads) *a_CH2OH | Sander et al. (2019) |
| G45029 | TrGCN | ISOPBNO3 + OH → ISOPBDNO3O2 | (k_adt+k_adp)*f_CH2ONO2 | Sander et al. (2019) |
| G45030 | TrGC | ISOPDO2 → .8 MACR + .8 HCHO + .8 $HO_2$ + .1 HCOC5 + .1 ISOPDOH | k1_RO2ISOPDO2 | Rickard and Pascoe (2009) |
| G45031a | TrGC | ISOPDO2 + $HO_2$ → ISOPDOOH | k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH) | Sander et al. (2019) |
| G45031b | TrGC | ISOPDO2 + $HO_2$ → MACR + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH | Sander et al. (2019) |
| G45032a | TrGCN | ISOPDO2 + NO → MACR + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(6,2,0,0,0, temp,cair)) | Lockwood et al. (2010), Sander et al. (2019) |
| G45032b | TrGCN | ISOPDO2 + NO → ISOPDNO3 | KRO2NO*alpha_AN(6,2,0,0,0,temp, cair) | Lockwood et al. (2010), Sander et al. (2019) |
| G45033 | TrGCN | ISOPDO2 + $NO_3$ → MACR + HCHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45034a | TrGC | ISOPDOOH + OH → LIEPOX + OH | (k_adt+k_adp)*a_CH2OOH | Paulot et al. (2009b), Sander et al. (2019) |
| G45034b | TrGC | ISOPDOOH + OH → ISOPDO2 | k_ROOHRO | Sander et al. (2019) |
| G45034c | TrGC | ISOPDOOH + OH → HCOC5 + OH | k_t*f_tOOH*f_allyl*f_pCH2OH | Sander et al. (2019) |
| G45034d | TrGC | ISOPDOOH + OH → $CH_3COCH_2OH$ + GLYOX + OH | k_s*f_pCH2OH*f_sOH | Sander et al. (2019) |
| G45035 | TrGC | ISOPDOOH + $O_3$ → 1.393 OH + BIACETOH + .67 HCHO + .05280 $HO_2$ + .2079 CO + .1221 $CH_2OO$ | 1.E-17 | Sander et al. (2019) |
| G45036 | TrGC | ISOPDOH + OH → HCOC5 + $HO_2$ | 2.*k_ROHRO+(k_t*f_tOH*f_allyl+k_ s*f_sOH)*f_pCH2OH+(k_adt+k_adp) *a_CH2OH | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45037 | TrGCN | ISOPDNO3 + OH → ISOPBDNO3O2 | (k_adp+k_ads)*a_CH2ONO2 | Sander et al. (2019)* |
| G45038 | TrGCN | NISOPO2 → .8 NC4CHO + .6 $HO_2$ + .2 LISOPACNO3 | k1_RO2LISOPACO2 | Rickard and Pascoe (2009) |
| G45039 | TrGCN | NISOPO2 + $HO_2$ → NISOPOOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009) |
| G45040 | TrGCN | NISOPO2 + NO → NC4CHO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45041 | TrGCN | NISOPO2 + $NO_3$ → NC4CHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45042 | TrGCN | NISOPOOH + OH → NC4CHO + OH | 1.03E-10 | Rickard and Pascoe (2009) |
| G45043 | TrGCN | NC4CHO + OH → LNISO3 | (k_adt+k_ads)*a_CHO*a_CH2ONO2 | Sander et al. (2019)* |
| G45044 | TrGCN | NC4CHO + $O_3$ → .27 NOA + .027 $HCOCO_2H$ + .0162 GLYOX + .0162 $H_2O_2$ + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 $NO_2$ + 0.7705 HCHO + .4055 $CO_2$ + .73 GLYOX | 2.40E-17 | Sander et al. (2019) |
| G45045 | TrGCN | NC4CHO + $NO_3$ → LNISO3 + $HNO_3$ | KNO3AL*4.25 | Rickard and Pascoe (2009) |
| G45046 | TrGCN | LNISO3 + $HO_2$ → LNISOOH | 0.5*k_RO2_HO2(temp,5)+0.5*KAPHO2 | Rickard and Pascoe (2009) |
| G45047 | TrGCN | LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 $HO_2$ + $NO_2$ + .5 $CO_2$ | 0.5*KAPNO+0.5*KRO2NO | Rickard and Pascoe (2009)* |
| G45048 | TrGCN | LNISO3 + $NO_3$ → NOA + .5 HOCHCHO + .5 CO + .5 $HO_2$ + $NO_2$ + .5 $CO_2$ | KRO2NO3*1.37 | Rickard and Pascoe (2009) |
| G45049 | TrGCN | LNISOOH + OH → LNISO3 | 2.65E-11 | Rickard and Pascoe (2009) |
| G45050a | TrGC | LHC4ACCHO + OH → LC578O2 | (k_adtertprim+k_ads)*a_CHO*a_CH2OH | Sander et al. (2019) |
| G45050b | TrGC | LHC4ACCHO + OH → LHC4ACCO3 | k_t*f_O | Sander et al. (2019) |
| G45050c | TrGC | LHC4ACCHO + OH → C4MDIAL + $HO_2$ | k_s*f_sOH*f_allyl | Sander et al. (2019) |
| G45051 | TrGC | LHC4ACCHO + $O_3$ → .2225 $CH_3C(O)$ + .89 CO + .0171875 $HOCH_2CO_2H$ + .075625 $H_2O_2$ + .0171875 $HCOCO_2H$ + .2775 $CH_3COCH_2OH$ + .6675 $HO_2$ + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 $HOCH_2CHO$ + .5 MGLYOX | 2.40E-17 | Rickard and Pascoe (2009) |
| G45052 | TrGCN | LHC4ACCHO + $NO_3$ → LHC4ACCO3 + $HNO_3$ | KNO3AL*4.25 | Rickard and Pascoe (2009) |
| G45053 | TrGC | LC578O2 → .25 $CH_3COCH_2OH$ + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 $HO_2$ | k1_RO2tORO2 | Rickard and Pascoe (2009) |
| G45054a | TrGC | LC578O2 + $HO_2$ → MGLYOX + $HOCH_2CHO$ + OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Rickard and Pascoe (2009) |
| G45054b | TrGC | LC578O2 + $HO_2$ → LC578OOH | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Rickard and Pascoe (2009) |
| G45055 | TrGCN | LC578O2 + NO → .25 $CH_3COCH_2OH$ + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45056 | TrGCN | LC578O2 + $NO_3$ → .25 $CH_3COCH_2OH$ + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45057 | TrGC | LC578O2 → .25 $CH_3COCH_2OH$ + .75 MGLYOX + .25 $HOCH_2CHO$ + .75 $HOCH_2CHO$ + $HO_2$ + OH | k_hsb | Sander et al. (2019) |
| G45058a | TrGC | LC578OOH + OH → LC578O2 | k_ROOHRO | Sander et al. (2019) |
| G45058b | TrGC | LC578OOH + OH → C1ODC2OOHC4OD + $HO_2$ | k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_pCH2OH*f_pCH2OH+k_s*f_sOH*f_pCH2OH | Sander et al. (2019) |
| G45059a | TrGC | LHC4ACCO3 → OH + .5 MACRO2 + .5 LHMVKABO2 + $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G45059b | TrGC | LHC4ACCO3 → LHC4ACCO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G45060a | TrGC | LHC4ACCO3 + $HO_2$ → 2 OH + .5 MACRO2 + .5 LHMVKABO2 + $CO_2$ | KAPHO2*r_CO3_OH | Sander et al. (2019) |
| G45060b | TrGC | LHC4ACCO3 + $HO_2$ → LHC4ACCO3H | KAPHO2*r_CO3_OOH | Sander et al. (2019) |
| G45060c | TrGC | LHC4ACCO3 + $HO_2$ → LHC4ACCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Sander et al. (2019) |
| G45061 | TrGCN | LHC4ACCO3 + NO → .5 MACRO2 + .5 LHMVKABO2 + $NO_2$ + $CO_2$ | KAPNO | Sander et al. (2019) |
| G45062 | TrGCN | LHC4ACCO3 + $NO_2$ → LC5PAN1719 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45063 | TrGCN | LHC4ACCO3 + $NO_3$ → .5 MACRO2 + .5 LHMVKABO2 + $NO_2$ + $CO_2$ | KRO2NO3*1.74 | Sander et al. (2019) |
| G45064a | TrGC | LHC4ACCO2H + OH → OH + .5 MACRO2 + .5 LHMVKABO2 + $CO_2$ | 2.52E-11 | Sander et al. (2019) |
| G45064b | TrGC | LHC4ACCO3H + OH → LHC4ACCO3 | 2.88E-11 | Rickard and Pascoe (2009) |
| G45065 | TrGCN | LC5PAN1719 → LHC4ACCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45066 | TrGCN | LC5PAN1719 + OH → .5 MACROH + .5 HO12CO3C4 + CO + $NO_2$ | 2.52E-11 | Rickard and Pascoe (2009) |
| G45067 | TrGC | HCOC5 + OH → C59O2 | 3.81E-11 | Rickard and Pascoe (2009) |
| G45068 | TrGC | HCOC5 + $O_3$ → BIACETOH + .335 $H_2O_2$ + .67 HCHO + .2079 CO + .1221 $CH_2OO$ + .05280 OH | 7.51E-16*EXP(-1521./temp) | Sander et al. (2019) |
| G45069 | TrGC | C59O2 → $CH_3COCH_2OH$ + HOCH2CO | k1_RO2tORO2 | Sander et al. (2019) |
| G45070a | TrGC | C59O2 + $HO_2$ → OH + $CH_3COCH_2OH$ + HOCH2CO | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Sander et al. (2019) |
| G45070b | TrGC | C59O2 + $HO_2$ → C59OOH | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Sander et al. (2019) |
| G45071 | TrGCN | C59O2 + NO → $CH_3COCH_2OH$ + HOCH2CO + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G45072 | TrGCN | C59O2 + $NO_3$ → $CH_3COCH_2OH$ + HOCH2CO + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G45073 | TrGC | C59OOH + OH → C59O2 | 9.7E-12 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45074 | TrGC | LIEPOX + OH → DB1O2 + $H_2O$ | 5.78E-11*EXP(-400./temp) *(1.52/3.+0.98*2./3.)/1.51 | Paulot et al. (2009b), Bates et al. (2014), Sander et al. (2019)* |
| G45075 | TrGC | ISOPBO2 → MVK + HCHO + OH | k_hsb | Sander et al. (2019) |
| G45076 | TrGC | ISOPDO2 → MACR + HCHO + OH | k_hsd | Sander et al. (2019) |
| G45077a | TrGC | LZCODC23DBCOOH + OH → .6 C1ODC2O2C4OOH + .4 C1OOHC2O2C4OD | k_adt*a_CHO*a_CH2OOH | Sander et al. (2019) |
| G45077b | TrGC | LZCODC23DBCOOH + OH → .6 C1ODC3O2C4OOH + .4 C1OOHC3O2C4OD | k_ads*a_CHO*a_CH2OOH | Sander et al. (2019) |
| G45077c | TrGC | LZCODC23DBCOOH + OH → LZCO3HC23DBCOD | k_t*f_O*f_alk+k_ROOHRO | Sander et al. (2019) |
| G45077d | TrGC | LZCODC23DBCOOH + OH → C4MDIAL + OH | k_s*f_sOOH*f_allyl | Sander et al. (2019) |
| G45078 | TrGC | LZCODC23DBCOOH + $O_3$ → .4672 OH + .2336 $HCOCOCH_2O_2$ + .2336 CO + .2336 $CH_3C(O)$ + .4672 HOOCH2CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH2CHO + .02765 $H_2O_2$ + .02592 $CH_3OOH$ + .02592 $CO_2$ + .01037 HCOCO + .01555 $CH_2OO$ + .01555 CO + .006908 $HOOCH_2CO_3$ + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 $HCOCOCH_2OOH$ + .2628 GLYOX + .0972 $CH_3COCH_2O_2H$ + .00972 $HCOCO_2H$ + .005832 GLYOX + .005832 $H_2O_2$ + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 $CO_2$ + .01458 HCOOH + .01458 CO | 2.4E-17 | Sander et al. (2019) |
| G45079 | TrGC | C1OOHC2O2C4OD → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH | k1_RO2tORO2 | Sander et al. (2019) |
| G45080 | TrGCN | C1OOHC2O2C4OD + NO → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G45081a | TrGC | C1OOHC2O2C4OD + $HO_2$ → C1OOHC2OOHC4OD | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Sander et al. (2019) |
| G45081b | TrGC | C1OOHC2O2C4OD + $HO_2$ → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + 1.22 OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Sander et al. (2019) |
| G45082 | TrGC | C1OOHC2O2C4OD → $CH_3COCH_2O_2H$ + GLYOX + OH | k_hsb | Sander et al. (2019) |
| G45083 | TrGC | C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD | k_15hsdhb | Sander et al. (2019) |
| G45084a | TrGC | C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH | 2.*k_s*f_sOOH*f_tCH2OH | Sander et al. (2019) |
| G45084b | TrGC | C1OOHC2OOHC4OD + OH → $CH_3COCH_2O_2H$ + 2 CO + 2 $HO_2$ + OH | k_t*f_tOH*f_pCH2OH*f_pCH2OH | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45084c | TrGC | C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD | k_ROOHRO | Sander et al. (2019) |
| G45085 | TrGC | C1ODC2OOHC4OD + OH → CO2H3CHO + CO + $H_2O$ + OH | k_t*f_O*f_tCH2OH+k_t*f_tOH*f_tOH*f_CHO | Sander et al. (2019) |
| G45086 | TrGC | C1ODC3O2C4OOH → MGLYOX + HOOCH2CHO + $HO_2$ | k1_RO2sORO2 | Sander et al. (2019) |
| G45087 | TrGCN | C1ODC3O2C4OOH + NO → MGLYOX + HOOCH2CHO + $HO_2$ + $NO_2$ | KRO2NO | Sander et al. (2019) |
| G45088 | TrGC | C1ODC3O2C4OOH + $HO_2$ → .5 $CH_3C(O)$ + .5 CO + .5 MGLYOX + .5 $HO_2$ + $HOOCH_2CO_3$ | k_RO2_HO2(temp,5) | Sander et al. (2019) |
| G45089 | TrGC | C1ODC3O2C4OOH → MGLYOX + OH + HOOCH2CHO | k_hsd | Sander et al. (2019) |
| G45090 | TrGC | C1OOHC3O2C4OD → .625 MGLYOX + 2 CO + 1.625 $HO_2$ + .375 $CH_3C(O)$ + .375 $CO_2$ + OH | k_15hsdhb | Sander et al. (2019) |
| G45091 | TrGC | LHC4ACCO3 → LZCO3HC23DBCOD + $HO_2$ | k_16hs | Sander et al. (2019) |
| G45092a | TrGC | C4MDIAL + OH → C1ODC2O2C4OD | (k_adt+k_ads)*a_CHO*a_CHO | Sander et al. (2019)* |
| G45092b | TrGC | C4MDIAL + OH → LZCO3C23DBCOD | 2.*k_t*f_O*f_alk | Sander et al. (2019)* |
| G45093 | TrGCN | C4MDIAL + $NO_3$ → LZCO3C23DBCOD + $HNO_3$ | KNO3AL*4.25*2. | Sander et al. (2019)* |
| G45094a | TrGC | C1ODC2O2C4OD + $HO_2$ → OH + MGLYOX + HOCHCHO | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Sander et al. (2019) |
| G45094b | TrGC | C1ODC2O2C4OD + $HO_2$ → C1ODC2OOHC4OD | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Sander et al. (2019) |
| G45095 | TrGCN | C1ODC2O2C4OD + NO → $NO_2$ + MGLYOX + HOCHCHO | KRO2NO | Sander et al. (2019)* |
| G45096 | TrGC | C1ODC2O2C4OD → MGLYOX + HOCHCHO | k1_RO2tORO2 | Sander et al. (2019) |
| G45097a | TrGC | C1ODC2OOHC4OD + OH → MGLYOX + 2 CO | (2.*k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_CHO*f_pCH2OH)*.5 | Sander et al. (2019) |
| G45097b | TrGC | C1ODC2OOHC4OD + OH → MGLYOX + 2 CO + OH | (2.*k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_CHO*f_pCH2OH)*.5 | Sander et al. (2019) |
| G45098 | TrGCN | LISOPACNO3O2 + NO → .21 NOA + .21 $HOCH_2CHO$ + .21 $HO_2$ + .49 HO12CO3C4 + .49 HCHO + .49 $NO_2$ + .045 MVKNO3 + .045 HCHO + .255 $CH_3COCH_2OH$ + .255 $NO_3$CH2CHO + .225 $H_2O_2$ + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G45099 | TrGCN | LISOPACNO3O2 → .21 NOA + .21 $HOCH_2CHO$ + .21 $HO_2$ + .49 HO12CO3C4 + .49 HCHO + .49 $NO_2$ + .045 MVKNO3 + .045 HCHO + .255 $CH_3COCH_2OH$ + .255 $NO_3$CH2CHO + .225 $H_2O_2$ | k1_RO2tORO2+k_RO2_HO2(temp,5)*c(ind_HO2) | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45100 | TrGCN | ISOPBDNO3O2 + NO → .6 $CH_3COCH_2OH$ + .6 $HOCH_2CHO$ + .26 MACRNO3 + .14 MVKNO3 + .4 HCHO + .4 $HO_2$ + 1.6 $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G45101 | TrGCN | ISOPBDNO3O2 → .6 $CH_3COCH_2OH$ + .6 $HOCH_2CHO$ + .26 MACRNO3 + .14 MVKNO3 + .4 HCHO + .4 $HO_2$ + .6 $NO_2$ | k1_RO2sORO2+k_RO2_HO2(temp,5) *c(ind_HO2) | Sander et al. (2019) |
| G45102 | TrGCN | LISOPACNO3 + $O_3$ → .8704 OH + .365 $HO_2$ + .73 MGLYOX + .4325 $NO_3$CH2CHO + .135 $CH_3COCH_2OH$ + .0675 GLYOX + .4325 $NO_2$ + .0891 $H_2O_2$ + .135 NOA + .0675 HOCHCHO + .3866 $HOCH_2CHO$ + .0405 $CH_3OH$ + .0405 CO + .0054 HOCH2CO | 2.8E-17 | Feierabend et al. (2008), Sander et al. (2019) |
| G45103 | TrGC | DB1O2 → DB1O2 | k1_RO2sORO2 | Sander et al. (2019) |
| G45104a | TrGC | DB1O2 + $HO_2$ → DB1OOH | k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH) | Sander et al. (2019)* |
| G45104b | TrGC | DB1O2 + $HO_2$ → DB1O2 + OH | k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH | Sander et al. (2019) |
| G45105a | TrGCN | DB1O2 + NO → DB1O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(7,2,0,0,0, temp,cair)) | Sander et al. (2019) |
| G45105b | TrGCN | DB1O2 + NO → DB1NO3 | KRO2NO*alpha_AN(7,2,0,0,0,temp, cair) | Sander et al. (2019) |
| G45106 | TrGCN | DB1O2 + $NO_3$ → DB1O2 + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G45107 | TrGC | DB1O2 → DB1O2 + OH | 1.E4 | Peeters and Nguyen (2012)* |
| G45108a | TrGC | DB1O2 → DB1O2 | KDEC*0.72 | see note* |
| G45108b | TrGC | DB1O2 → .5 HVMK + .5 HMAC + HCHO + $HO_2$ | KDEC*0.28 | see note* |
| G45109 | TrGC | DB1O2 → .48 $CH_3COCH_2OH$ + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + $HO_2$ | k1_RO2sORO2 | Sander et al. (2019) |
| G45110a | TrGC | DB1O2 + $HO_2$ → DB2OOH | k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH) | Sander et al. (2019) |
| G45110b | TrGC | DB1O2 + $HO_2$ → .48 $CH_3COCH_2OH$ + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + $HO_2$ + OH | k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH | Sander et al. (2019) |
| G45111 | TrGCN | DB1O2 + NO → .48 $CH_3COCH_2OH$ + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + $HO_2$ + $NO_2$ | KRO2NO | see note* |
| G45112 | TrGCN | DB1O2 + $NO_3$ → .48 $CH_3COCH_2OH$ + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + $HO_2$ + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G45113 | TrGC | DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH | k_14hsal | Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45114a | TrGC | DB1OOH + OH → DB1O2 | k_ROOHRO | Sander et al. (2019) |
| G45114b | TrGC | DB1OOH + OH → HCOOH + $HO_2$ + $CH_3COCHO_2CHO$ | k_adt | Sander et al. (2019)* |
| G45115 | TrGC | DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH | 4.67E-26*(temp)**(3.286) *EXP(4509./(1.987*temp)) | Sander et al. (2019), da Silva (2010)* |
| G45116 | TrGCN | DB1NO3 + OH → HCOOH + $NO_2$ + $CH_3COCHO_2CHO$ | k_adt | Sander et al. (2019)* |
| G45117 | TrGC | DB2OOH + OH → DB1O2 | k_ROOHRO | Sander et al. (2019)* |
| G45118 | TrGC | LISOPACOOH + $O_3$ → 1.3272 OH + .36986 $HO_2$ + .0432 $H_2O_2$ + .08422 CO + .2025 $CH_3OOH$ + .01215 $CH_2OO$ + .3704 HCHO + .00405 $CH_3OH$ + .0405 $CO_2$ + .1825 HOCH2COCH2O2 + .365 MGLYOX + .3866 HOOCH2CHO + .135 $CH_3COCH_2OH$ + .0675 GLYOX + .00324 HCOCO + .3866 $HOCH_2CHO$ + .135 $CH_3COCH_2O_2H$ + .0675 HOCHCHO + .0054 HOCH2CO | 4.829E-16 | Sander et al. (2019) |
| G45119a | TrGC | LZCO3HC23DBCOD + OH → .62 CO2H3CHO + .62 OH + .62 $CO_2$ + .38 MGLYOX + .38 $HCOCO_3H$ + .38 $HO_2$ | k_adt*a_CHO*a_CO2H | Sander et al. (2019) |
| G45119b | TrGC | LZCO3HC23DBCOD + OH → .62 $CH_3COCO_3H$ + 1.24 CO + 1.24 $HO_2$ + .38 MGLYOX + .38 $HO_2$ + .38 CO + .38 $HO_2$ + .38 OH + .38 $CO_2$ | k_ads*a_CHO*a_CO2H | Sander et al. (2019) |
| G45120 | TrGC | LISOPEFO2 → LISOPEFO | k1_RO2pORO2 | Sander et al. (2019) |
| G45121a | TrGCN | LISOPEFO2 + NO → LISOPEFO + $NO_2$ | KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair)) | Sander et al. (2019) |
| G45121b | TrGCN | LISOPEFO2 + NO → ISOPDNO3 | KRO2NO*alpha_AN(6,1,0,0,0,temp, cair) | Sander et al. (2019)* |
| G45122a | TrGC | LISOPEFO2 + $HO_2$ → .7143 ISOPDOOH + .2857 ISOPBOOH | k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH) | Sander et al. (2019) |
| G45122b | TrGC | LISOPEFO2 + $HO_2$ → LISOPEFO + OH | k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH | Sander et al. (2019) |
| G45123 | TrGCN | LISOPEFO2 + $NO_3$ → LISOPEFO + $NO_2$ | KRO2NO3 | Sander et al. (2019) |
| G45124 | TrGC | LISOPEFO2 → .7143 MACR + .2857 MVK + HCHO + OH | 0.7143*k_hsd+.2857*k_hsb | Sander et al. (2019) |
| G45125 | TrGC | LISOPEFO → .7143 MACR + .2857 MVK + HCHO + $HO_2$ | KDEC | Sander et al. (2019) |
| G45126a | TrGC | LISOPACO → 3METHYLFURAN + $HO_2$ | KDEC*0.37 | Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45126b | TrGC | LISOPACO → .65 LHC4ACCHO + .65 $HO_2$ + .35 DB1O2 | KDEC*(1.-0.37) | Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45127a | TrGC | LISOPACO → 3METHYLFURAN + $HO_2$ | KDEC*0.37 | Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45127b | TrGC | LISOPACO → .65 LHC4ACCHO + .65 $HO_2$ + .35 DB1O2 | KDEC*(1.-0.37) | Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45128 | TrGC | 3METHYLFURAN + OH → L3METHYLFURANO2 | 3.2E-11*EXP(310./temp) | Sander et al. (2019)* |
| G45129 | TrGCN | 3METHYLFURAN + $NO_3$ → L3METHYLFURANO2 + $NO_2$ | 1.9E-11 | Sander et al. (2019), Atkinson et al. (2006)* |
| G45130 | TrGC | L3METHYLFURANO2 → C4MDIAL + $HO_2$ | k1_RO2sORO2 | Sander et al. (2019) |
| G45131 | TrGCN | L3METHYLFURANO2 + NO → C4MDIAL + $HO_2$ + $NO_2$ | KRO2NO | Sander et al. (2019)* |
| G45132 | TrGC | L3METHYLFURANO2 + $HO_2$ → C4MDIAL + $HO_2$ | k_RO2_HO2(temp,5) | Sander et al. (2019)* |
| G45133 | TrGC | LZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + $CO_2$ | k1_RO2RCO3 | Sander et al. (2019) |
| G45134a | TrGC | LZCO3C23DBCOD + $HO_2$ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Sander et al. (2019) |
| G45134b | TrGC | LZCO3C23DBCOD + $HO_2$ → LZCO3HC23DBCOD | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Sander et al. (2019)* |
| G45135 | TrGCN | LZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + $CO_2$ + $NO_2$ | KAPNO | Sander et al. (2019) |
| G45136 | TrGCN | LZCO3C23DBCOD + $NO_2$ → LZCPANC23DBCOD | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45137 | TrGCN | LZCO3C23DBCOD + $NO_3$ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Sander et al. (2019) |
| G45138 | TrGCN | LZCPANC23DBCOD → LZCO3C23DBCOD + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45139 | TrGCN | LZCPANC23DBCOD + OH → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + $CO_2$ + $NO_2$ | 2.52E-11 | Sander et al. (2019)* |
| G45200 | TrGTerC | C511O2 → $CH_3C(O)$ + HCOCH2CHO | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G45201 | TrGTerCN | C511O2 + NO → $CH_3C(O)$ + HCOCH2CHO + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45202a | TrGTerC | C511O2 + $HO_2$ → C511OOH | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45202b | TrGTerC | C511O2 + $HO_2$ → $CH_3C(O)$ + HCOCH2CHO + OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45203 | TrGTerC | C511OOH + OH → C511O2 | 7.49E-11 | Rickard and Pascoe (2009) |
| G45204 | TrGTerC | CO23C4CHO + OH → CO23C4CO3 | 6.65E-11 | Rickard and Pascoe (2009) |
| G45205 | TrGTerCN | CO23C4CHO + $NO_3$ → CO23C4CO3 + $HNO_3$ | KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G45206 | TrGTerC | CO23C4CO3 → $CH_3COCOCH_2O_2$ + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G45207 | TrGTerCN | CO23C4CO3 + NO → $CH_3COCOCH_2O_2$ + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G45208 | TrGTerCN | CO23C4CO3 + $NO_2$ → C5PAN9 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45209a | TrGTerC | CO23C4CO3 + $HO_2$ → CO23C4CO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G45209b | TrGTerC | CO23C4CO3 + $HO_2$ → $CH_3COCOCH_2O_2$ + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G45210 | TrGTerCN | C5PAN9 → CO23C4CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45211 | TrGTerCN | C5PAN9 + OH → $CH_3COCOCHO$ + CO + $NO_2$ | 3.12E-13 | Rickard and Pascoe (2009) |
| G45212 | TrGTerC | C512O2 → C513O2 | k1_RO2pRO2 | Rickard and Pascoe (2009) |
| G45213 | TrGTerC | C512O2 + $HO_2$ → C512OOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009) |
| G45214 | TrGTerCN | C512O2 + NO → C513O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45215 | TrGTerC | C512OOH + OH → CO13C4CHO + OH | 1.01E-10 | Rickard and Pascoe (2009) |
| G45216 | TrGTerC | C513O2 → GLYOX + $HOC_2H_4CO_3$ | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G45217 | TrGTerCN | C513O2 + NO → GLYOX + $HOC_2H_4CO_3$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45218a | TrGTerC | C513O2 + $HO_2$ → C513OOH | k_RO2_HO2(temp,5)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45218b | TrGTerC | C513O2 + $HO_2$ → GLYOX + $HOC_2H_4CO_3$ + OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45219 | TrGTerC | CO13C4CHO + OH → CHOC3COCO3 | 1.33E-10 | Rickard and Pascoe (2009) |
| G45220 | TrGTerCN | CO13C4CHO + $NO_3$ → CHOC3COCO3 + $HNO_3$ | 2.*KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G45221 | TrGTerC | C513OOH + OH → C513CO + OH | 9.23E-11 | Rickard and Pascoe (2009) |
| G45222 | TrGTerC | CHOC3COCO3 → CHOC3COO2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G45223 | TrGTerC | CHOC3COCO3 + $HO_2$ → CHOC3COOOH | KAPHO2 | Rickard and Pascoe (2009) |
| G45224 | TrGTerCN | CHOC3COCO3 + $NO_2$ → CHOC3COPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45225 | TrGTerCN | CHOC3COCO3 + NO → CHOC3COO2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G45226 | TrGTerC | C513CO + OH → $HOC_2H_4CO_3$ + CO + CO | 2.64E-11 | Rickard and Pascoe (2009) |
| G45227 | TrGTerC | C514O2 + $HO_2$ → C514OOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009) |
| G45228a | TrGTerCN | C514O2 + NO → CO13C4CHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(7,2,0,1,0, temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45228b | TrGTerCN | C514O2 + NO → C514NO3 | KRO2NO*alpha_AN(7,2,0,1,0,temp, cair) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45229 | TrGTerCN | C514O2 + $NO_3$ → CO13C4CHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G45230 | TrGTerC | C514O2 → CO13C4CHO + $HO_2$ | k1_RO2sRO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45231 | TrGTerC | C514OOH + OH → CO13C4CHO + OH | 1.10E-10 | Rickard and Pascoe (2009) |
| G45232 | TrGTerCN | C514NO3 + OH → CO13C4CHO + $NO_2$ | 4.33E-11 | Rickard and Pascoe (2009) |
| G45233 | TrGTerC | CHOC3COOOH + OH → CHOC3COCO3 | 7.55E-11 | Rickard and Pascoe (2009) |
| G45234 | TrGTerCN | CHOC3COPAN → CHOC3COCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45235 | TrGTerCN | CHOC3COPAN + OH → C4CODIAL + CO + $NO_2$ | 7.19E-11 | Rickard and Pascoe (2009) |
| G45236 | TrGTerC | MBO + OH → LMBOABO2 | 8.1E-12*EXP(610./temp) | Rickard and Pascoe (2009), Sander et al. (2019)* |
| G45237a | TrGTerC | MBO + $O_3$ → HCHO + .16 $CH_3COCH_3$ + .16 $HO_2$ + .16 CO + .16 OH + .84 MBOOO | 1.0E-17*0.57 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45237b | TrGTerC | MBO + $O_3$ → IBUTALOH + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 $HO_2$ | 1.0E-17*0.43 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45238 | TrGTerCN | MBO + $NO_3$ → LNMBOABO2 | 4.6E-14*EXP(-400./temp) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45239 | TrGTerC | LMBOABO2 + $HO_2$ → LMBOABOOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45240a | TrGTerCN | LMBOABO2 + NO → LMBOABNO3 | KRO2NO*(.67*alpha_AN(7,2,0,0,0, temp,cair)+.33*alpha_AN(7,1,0,0, 0,temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45240b | TrGTerCN | LMBOABO2 + NO → $HOCH_2CHO$ + $CH_3COCH_3$ + $HO_2$ + $NO_2$ | KRO2NO*(1.-(.67*alpha_AN(7,2,0, 0,0,temp,cair)+.33*alpha_AN(7,1, 0,0,0,temp,cair)))*.67 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45240c | TrGTerCN | LMBOABO2 + NO → IBUTALOH + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-(.67*alpha_AN(7,2,0, 0,0,temp,cair)+.33*alpha_AN(7,1, 0,0,0,temp,cair)))*.33 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45241a | TrGTerC | LMBOABO2 → $HOCH_2CHO$ + $CH_3COCH_3$ + $HO_2$ | k1_RO2sORO2*.67 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45241b | TrGTerC | LMBOABO2 → IBUTALOH + HCHO + $HO_2$ | k1_RO2pORO2*.33 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45242a | TrGTerC | LMBOABOOH + OH → MBOACO | 0.67*2.93E-11+.33*2.05E-12 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45242b | TrGTerC | LMBOABOOH + OH → LMBOABO2 | k_ROOHRO | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45243 | TrGTerCN | LMBOABNO3 + OH → MBOACO + $NO_2$ | 0.67*1.75E-12+.33*2.69E-12 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45244 | TrGTerC | MBOACO + OH → MBOCOCO + $HO_2$ | 3.79E-12 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45245 | TrGTerC | MBOCOCO + OH → CO + IPRHOCO3 | 1.38E-11 | Rickard and Pascoe (2009) |
| G45246 | TrGTerCN | LNMBOABO2 + $HO_2$ → LNMBOABOOH | k_RO2_HO2(temp,5) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45247 | TrGTerCN | LNMBOABO2 + NO → .65 $NO_3$CH2CHO + .65 $CH_3COCH_3$ + .65 $HO_2$ + .35 IBUTALOH + .35 HCHO + .35 $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009), Sander et al. (2019)* |
| G45248 | TrGTerCN | LNMBOABO2 + $NO_3$ → .65 $NO_3$CH2CHO + .65 $CH_3COCH_3$ + .65 $HO_2$ + .35 IBUTALOH + .35 HCHO + .35 $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45249 | TrGTerCN | LNMBOABO2 → .65 $NO_3$CH2CHO + .65 $CH_3COCH_3$ + .65 $HO_2$ + .35 IBUTALOH + .35 HCHO + .35 $NO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45250a | TrGTerCN | LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBCO | 0.65*4.89E-12+.35*2.52E-12 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45250b | TrGTerCN | LNMBOABOOH + OH → LNMBOABO2 | k_ROOHRO | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45251 | TrGTerCN | NMBOBCO + OH → NC4OHCO3 | 4.26E-12 | Rickard and Pascoe (2009) |
| G45252a | TrGTerCN | NC4OHCO3 + $HO_2$ → IBUTALOH + $CO_2$ + $NO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45252b | TrGTerCN | NC4OHCO3 + $HO_2$ → NC4OHCO3H | KAPHO2*(r_CO3_O3+r_CO3_OOH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45253 | TrGTerCN | NC4OHCO3 + NO → IBUTALOH + $CO_2$ + $NO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G45254 | TrGTerCN | NC4OHCO3 + $NO_2$ → NC4OHCPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45255 | TrGTerCN | NC4OHCO3 + $NO_3$ → IBUTALOH + $CO_2$ + $NO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G45256 | TrGTerCN | NC4OHCO3 → IBUTALOH + $CO_2$ + $NO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G45257 | TrGTerCN | NC4OHCO3H + OH → NC4OHCO3 | 4.50E-12 | Rickard and Pascoe (2009) |
| G45258 | TrGTerCN | NC4OHCPAN + OH → IBUTALOH + CO + $NO_2$ + $NO_2$ | 1.27E-12 | Rickard and Pascoe (2009) |
| G45259 | TrGTerCN | NC4OHCPAN → NC4OHCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45260 | TrGTerCN | C4MCONO3OH + OH → $CH_3COCH_3$ + HCHO + $CO_2$ + $NO_2$ | 1.23E-12 | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45400 | TrGAroCN | NC4MDCO2HN + OH → MMALANHY + $NO_2$ | k_ROOHRO | Rickard and Pascoe (2009)* |
| G45401 | TrGAroCN | C54CO + $NO_3$ → 3 CO + $CH_3C(O)OO$ + $HNO_3$ | KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G45402 | TrGAroC | C54CO + OH → 3 CO + $CH_3C(O)OO$ | 1.72E-11 | Rickard and Pascoe (2009) |
| G45403a | TrGAroCN | NTLFUO2 + $HO_2$ → NTLFUOOH | k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G45403b | TrGAroCN | NTLFUO2 + $HO_2$ → ACCOMECHO + $NO_2$ + OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45404 | TrGAroCN | NTLFUO2 + NO → ACCOMECHO + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45405 | TrGAroCN | NTLFUO2 + $NO_3$ → ACCOMECHO + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G45406 | TrGAroCN | NTLFUO2 → ACCOMECHO + $NO_2$ | k1_RO2tORO2 | Rickard and Pascoe (2009)* |
| G45407 | TrGAroC | C5134CO2OH + OH → C54CO + $HO_2$ | 7.48E-11 | Rickard and Pascoe (2009) |
| G45408 | TrGAroCN | C5COO2NO2 + OH → MGLYOX + CO + CO + $NO_2$ | 5.43E-11 | Rickard and Pascoe (2009) |
| G45409 | TrGAroCN | C5COO2NO2 → C5CO14O2 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009)* |
| G45410 | TrGAroC | C5DIALOOH + OH → C5DIALCO + OH | 7.52E-11 | Rickard and Pascoe (2009) |
| G45411a | TrGAroC | C4CO2DBCO3 + $HO_2$ → C4CO2DCO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G45411b | TrGAroC | C4CO2DBCO3 + $HO_2$ → $HO_2$ + CO + HCOCOCHO + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45412 | TrGAroCN | C4CO2DBCO3 + NO → $HO_2$ + CO + HCOCOCHO + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G45413 | TrGAroCN | C4CO2DBCO3 + $NO_2$ → C4CO2DBPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G45414 | TrGAroCN | C4CO2DBCO3 + $NO_3$ → $HO_2$ + CO + HCOCOCHO + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G45415 | TrGAroC | C4CO2DBCO3 → $HO_2$ + CO + HCOCOCHO + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G45416 | TrGAroC | MMALANHY + OH → MMALANHYO2 | 1.50E-12 | Rickard and Pascoe (2009) |
| G45421a | TrGAroC | MMALANHYO2 + $HO_2$ → MMALNHYOOH | k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45421b | TrGAroC | MMALANHYO2 + $HO_2$ → CO2H3CO3 + $CO_2$ + OH | k_RO2_HO2(temp,5)*(r_COCH2O2_OH+r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G45422 | TrGAroCN | MMALANHYO2 + NO → CO2H3CO3 + $CO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45423 | TrGAroCN | MMALANHYO2 + $NO_3$ → CO2H3CO3 + $CO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G45424 | TrGAroC | MMALANHYO2 → CO2H3CO3 + $CO_2$ | k1_RO2tORO2 | Rickard and Pascoe (2009)* |
| G45428 | TrGAroCN | C4CO2DBPAN + OH → HCOCOCHO + $CO_2$ + CO + $NO_2$ | 2.74E-11 | Rickard and Pascoe (2009) |
| G45429 | TrGAroCN | C4CO2DBPAN → C4CO2DBCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009)* |
| G45430a | TrGAroC | C5CO14O2 + $HO_2$ → .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009)* |
| G45430b | TrGAroC | C5CO14O2 + $HO_2$ → C5CO14OH + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G45430c | TrGAroC | C5CO14O2 + $HO_2$ → C5CO14OOH | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G45431 | TrGAroCN | C5CO14O2 + NO → .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G45432 | TrGAroCN | C5CO14O2 + $NO_2$ → C5COO2NO2 | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45433 | TrGAroCN | C5CO14O2 + $NO_3$ → .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009)* |
| G45434 | TrGAroC | C5CO14O2 → .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G45436 | TrGAroC | C5CO14OH + OH → .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ | 5.44E-11 | Rickard and Pascoe (2009)* |
| G45441 | TrGAroCN | C5DICARB + $NO_3$ → C5CO14O2 + $HNO_3$ | KNO3AL*2.75 | Rickard and Pascoe (2009) |
| G45442 | TrGAroC | C5DICARB + $O_3$ → .5338 GLYOX + .063 $CH_3CHO$ + .348 $CH_3C(O)OO$ + .918 CO + .57 OH + .473 $HO_2$ + .0563 $CH_3COCO_2H$ + .5338 MGLYOX + .676 $H_2O_2$ + .063 HCHO + .0563 $HCOCO_2H$ + .2465 $CO_2$ | 2.00E-18 | Rickard and Pascoe (2009) |
| G45443 | TrGAroC | C5DICARB + OH → .48 C5CO14O2 + .52 C5DICARBO2 | 6.2E-11 | Rickard and Pascoe (2009) |
| G45444 | TrGAroC | MC3ODBCO2H + OH → .35 GLYOX + .35 $CH_3$ + .35 CO + .35 $CO_2$ + .65 MMALANHY + .65 $HO_2$ | 4.38E-11 | Rickard and Pascoe (2009)* |
| G45451 | TrGAroCN | TLFUONE + $NO_3$ → NTLFUO2 | 1.00E-12 | Rickard and Pascoe (2009) |
| G45452 | TrGAroC | TLFUONE + $O_3$ → .5 CO + .5 OH + .5 MECOACETO2 + .3125 C24O3CCO2H + .1875 ACCOMECHO + .1875 $H_2O_2$ | 8.00E-19 | see note* |
| G45453 | TrGAroC | TLFUONE + OH → TLFUO2 | 6.90E-11 | Rickard and Pascoe (2009) |
| G45454a | TrGAroC | ACCOMECO3 + $HO_2$ → ACCOMECO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G45454b | TrGAroC | ACCOMECO3 + $HO_2$ → MECOACETO2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G45455 | TrGAroCN | ACCOMECO3 + NO → MECOACETO2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G45456 | TrGAroCN | ACCOMECO3 + $NO_2$ → ACCOMEPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G45457 | TrGAroCN | ACCOMECO3 + $NO_3$ → MECOACETO2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G45458 | TrGAroC | ACCOMECO3 → MECOACETO2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G45459 | TrGAroC | C4CO2DCO3H + OH → C4CO2DBCO3 | 3.06E-11 | Rickard and Pascoe (2009) |
| G45464 | TrGAroCN | ACCOMECHO + $NO_3$ → ACCOMECO3 + $HNO_3$ | KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G45465 | TrGAroC | ACCOMECHO + OH → ACCOMECO3 | 7.09E-11 | Rickard and Pascoe (2009) |
| G45466 | TrGAroC | MMALNHYOOH + OH → MMALANHYO2 | 1.69E-11 | Rickard and Pascoe (2009) |
| G45467a | TrGAroC | C5DICAROOH + OH → C5134CO2OH + OH | 1.21E-10 | Rickard and Pascoe (2009) |
| G45467b | TrGAroC | C5DICAROOH + OH → C5DICARBO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G45468 | TrGAroC | C24O3CCO2H + OH → MECOACETO2 + $CO_2$ | 8.76E-13 | Rickard and Pascoe (2009) |
| G45469 | TrGAroCN | NTLFUOOH + OH → NTLFUO2 | 4.44E-12 | Rickard and Pascoe (2009) |
| G45470 | TrGAroCN | ACCOMEPAN + OH → METACETHO + CO + CO + $NO_2$ | 1.00E-14 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G45471 | TrGAroCN | ACCOMEPAN → ACCOMECO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45476a | TrGAroC | TLFUO2 + $HO_2$ → TLFUOOH | k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G45476b | TrGAroC | TLFUO2 + $HO_2$ → ACCOMECHO + $HO_2$ + OH | k_RO2_HO2(temp,5)*(r_COCH2O2_OH+r_CHOHCH2O2_OH) | Rickard and Pascoe (2009)* |
| G45477 | TrGAroCN | TLFUO2 + NO → ACCOMECHO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45478 | TrGAroCN | TLFUO2 + $NO_3$ → ACCOMECHO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G45479 | TrGAroC | TLFUO2 → ACCOMECHO + $HO_2$ | k1_RO2tORO2 | Rickard and Pascoe (2009)* |
| G45480 | TrGAroC | C5CO14OOH + OH → C5CO14O2 | 3.59E-12 | Rickard and Pascoe (2009) |
| G45483 | TrGAroC | TLFUOOH + OH → TLFUO2 | 2.53E-11 | Rickard and Pascoe (2009) |
| G45485 | TrGAroC | ACCOMECO3H + OH → ACCOMECO3 | 3.59E-12 | Rickard and Pascoe (2009) |
| G45486a | TrGAroC | C5DIALO2 + $HO_2$ → C5DIALOOH | k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G45486b | TrGAroC | C5DIALO2 + $HO_2$ → MALDIAL + CO + $HO_2$ + OH | k_RO2_HO2(temp,5)*r_COCH2O2_OH | Rickard and Pascoe (2009)* |
| G45487 | TrGAroCN | C5DIALO2 + NO → MALDIAL + CO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45488 | TrGAroCN | C5DIALO2 + $NO_3$ → MALDIAL + CO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G45489 | TrGAroC | C5DIALO2 → MALDIAL + CO + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G45490a | TrGAroC | C5DICARBO2 + $HO_2$ → C5DICAROOH | k_RO2_HO2(temp,5)*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G45491b | TrGAroC | C5DICARBO2 + $HO_2$ → MGLYOX + GLYOX + $HO_2$ + OH | k_RO2_HO2(temp,5)*r_CO3_OH | Rickard and Pascoe (2009)* |
| G45492 | TrGAroCN | C5DICARBO2 + NO → MGLYOX + GLYOX + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G45493 | TrGAroCN | C5DICARBO2 + $NO_3$ → MGLYOX + GLYOX + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G45494 | TrGAroC | C5DICARBO2 → MGLYOX + GLYOX + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G46200a | TrGTerC | CO235C6O2 + $HO_2$ → CO235C6OOH | k_RO2_HO2(temp,6)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G46200b | TrGTerC | CO235C6O2 + $HO_2$ → CO23C4CO3 + HCHO + OH | k_RO2_HO2(temp,6)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G46201 | TrGTerCN | CO235C6O2 + NO → CO23C4CO3 + HCHO + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46202 | TrGTerC | CO235C6O2 → CO23C4CO3 + HCHO | k1_RO2pORO2 | Rickard and Pascoe (2009) |
| G46203 | TrGTerC | CO235C6OOH + OH → CO235C6O2 | 1.01E-11 | Rickard and Pascoe (2009) |
| G46204 | TrGTerC | C614O2 → CO23C4CHO + HCHO + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46205a | TrGTerCN | C614O2 + NO $\rightarrow$ CO23C4CHO + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(9,2,0,1,0, temp,cair)) | Rickard and Pascoe (2009) |
| G46205b | TrGTerCN | C614O2 + NO $\rightarrow$ C614NO3 | KRO2NO*alpha_AN(9,2,0,1,0,temp, cair) | Rickard and Pascoe (2009) |
| G46206a | TrGTerC | C614O2 + $HO_2$ $\rightarrow$ C614OOH | k_RO2_HO2(temp,6)*(1.-r_ CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G46206b | TrGTerC | C614O2 + $HO_2$ $\rightarrow$ CO23C4CHO + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G46207 | TrGTerCN | C614NO3 + OH $\rightarrow$ C614CO + $NO_2$ | 7.11E-12 | Rickard and Pascoe (2009) |
| G46208 | TrGTerC | C614OOH + OH $\rightarrow$ C614CO + OH | 8.69E-11 | Rickard and Pascoe (2009) |
| G46209 | TrGTerC | C614CO + OH $\rightarrow$ CO235C5CHO + $HO_2$ | 3.22E-12 | Rickard and Pascoe (2009) |
| G46210 | TrGTerC | CO235C5CHO + OH $\rightarrow$ CO23C4CO3 + CO | 1.33E-11 | Rickard and Pascoe (2009) |
| G46211 | TrGTerCN | CO235C5CHO + $NO_3$ $\rightarrow$ CO23C4CO3 + CO + $HNO_3$ | KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G46400 | TrGAroC | PHENOOH + OH $\rightarrow$ PHENO2 | 1.16E-10 | Rickard and Pascoe (2009) |
| G46401 | TrGAroC | C6CO4DB + OH $\rightarrow$ CO + CO + $HO_2$ + CO + HCOCOCHO | 7.70E-11 | Rickard and Pascoe (2009) |
| G46402 | TrGAroC | C5CO2DCO3H + OH $\rightarrow$ C5CO2DBCO3 | 3.60E-11 | Rickard and Pascoe (2009) |
| G46403 | TrGAroCN | NDNPHENOOH + OH $\rightarrow$ NDNPHENO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G46404a | TrGAroC | C615CO2O2 + $HO_2$ $\rightarrow$ C615CO2OOH | k_RO2_HO2(temp,6)*(1.-r_COCH2O2_ OH) | Rickard and Pascoe (2009) |
| G46404b | TrGAroC | C615CO2O2 + $HO_2$ $\rightarrow$ C5DICARB + CO + $HO_2$ + OH | k_RO2_HO2(temp,6)*r_COCH2O2_OH | Rickard and Pascoe (2009)* |
| G46405 | TrGAroCN | C615CO2O2 + NO $\rightarrow$ C5DICARB + CO + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46406 | TrGAroCN | C615CO2O2 + $NO_3$ $\rightarrow$ C5DICARB + CO + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46407 | TrGAroC | C615CO2O2 $\rightarrow$ C5DICARB + CO + $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G46408 | TrGAroCN | BZEMUCPAN + OH $\rightarrow$ MALDIAL + CO + $CO_2$ + $NO_2$ | 4.05E-11 | Rickard and Pascoe (2009) |
| G46409 | TrGAroCN | BZEMUCPAN $\rightarrow$ BZEMUCCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G46410 | TrGAroCN | BZBIPERNO3 + OH $\rightarrow$ BZOBIPEROH + $NO_2$ | 7.30E-11 | Rickard and Pascoe (2009) |
| G46411 | TrGAroCN | HOC6H4NO2 + $NO_3$ $\rightarrow$ NPHEN1O + $HNO_3$ | 9.00E-14 | Rickard and Pascoe (2009) |
| G46412 | TrGAroCN | HOC6H4NO2 + OH $\rightarrow$ NPHEN1O | 9.00E-13 | Rickard and Pascoe (2009) |
| G46413a | TrGAroCN | NDNPHENO2 + $HO_2$ $\rightarrow$ NDNPHENOOH | k_RO2_HO2(temp,6)*(1.-r_ CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46413b | TrGAroCN | NDNPHENO2 + $HO_2$ $\rightarrow$ NC4DCO2H + $HNO_3$ + CO + CO + $NO_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46414 | TrGAroCN | NDNPHENO2 + NO $\rightarrow$ NC4DCO2H + $HNO_3$ + CO + CO + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46415 | TrGAroCN | NDNPHENO2 + $NO_3$ → NC4DCO2H + $HNO_3$ + CO + CO + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46416 | TrGAroCN | NDNPHENO2 → NC4DCO2H + $HNO_3$ + CO + CO + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46417 | TrGAroC | PBZQCO + OH → C5CO2OHCO3 | 6.07E-11 | Rickard and Pascoe (2009) |
| G46418 | TrGAroCN | CATECHOL + $NO_3$ → CATEC1O + $HNO_3$ | 9.9E-11 | Rickard and Pascoe (2009)* |
| G46419 | TrGAroC | CATECHOL + $O_3$ → MALDALCO2H + $HCOCO_2H$ + $HO_2$ + OH | 9.2E-18 | Rickard and Pascoe (2009) |
| G46420 | TrGAroC | CATECHOL + OH → CATEC1O | 1.0E-10 | Rickard and Pascoe (2009) |
| G46421 | TrGAroC | C5COOHCO3H + OH → C5CO2OHCO3 | 8.01E-11 | Rickard and Pascoe (2009) |
| G46422 | TrGAroCN | NCATECHOL + $NO_3$ → NNCATECO2 | 2.60E-12 | Rickard and Pascoe (2009) |
| G46423 | TrGAroCN | NCATECHOL + OH → NCATECO2 | 3.47E-12 | Rickard and Pascoe (2009) |
| G46424a | TrGAroC | C5CO2OHCO3 + $HO_2$ → C5COOHCO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G46424b | TrGAroC | C5CO2OHCO3 + $HO_2$ → HOCOC4DIAL + $HO_2$ + CO + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G46425 | TrGAroCN | C5CO2OHCO3 + NO → HOCOC4DIAL + $HO_2$ + CO + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G46426 | TrGAroCN | C5CO2OHCO3 + $NO_2$ → C5CO2OHPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G46427 | TrGAroCN | C5CO2OHCO3 + $NO_3$ → HOCOC4DIAL + $HO_2$ + CO + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G46428 | TrGAroC | C5CO2OHCO3 → HOCOC4DIAL + $HO_2$ + CO + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G46429 | TrGAroCN | BZEPOXMUC + $NO_3$ → BZEMUCCO3 + $HNO_3$ | 2.*KNO3AL*2.75 | Rickard and Pascoe (2009) |
| G46430 | TrGAroC | BZEPOXMUC + $O_3$ → EPXC4DIAL + .125 HCHO + .1125 $HCOCO_2H$ + .0675 GLYOX + .0675 $H_2O_2$ + .82 $HO_2$ + .57 OH + 1.265 CO + .25 $CO_2$ | 2.00E-18 | Rickard and Pascoe (2009)* |
| G46431 | TrGAroC | BZEPOXMUC + OH → .31 BZEMUCCO3 + .69 BZEMUCO2 | 6.08E-11 | Rickard and Pascoe (2009) |
| G46432a | TrGAroCN | NCATECO2 + $HO_2$ → NCATECOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46432b | TrGAroCN | NCATECO2 + $HO_2$ → NC4DCO2H + $HCOCO_2H$ + $HO_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46433 | TrGAroCN | NCATECO2 + NO → NC4DCO2H + $HCOCO_2H$ + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46434 | TrGAroCN | NCATECO2 + $NO_3$ → NC4DCO2H + $HCOCO_2H$ + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46435 | TrGAroCN | NCATECO2 → NC4DCO2H + HCOCO$_2$H + HO$_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46436 | TrGAroCN | NPHEN1OOH + OH → NPHEN1O2 | 9.00E-13 | Rickard and Pascoe (2009) |
| G46437a | TrGAroCN | NPHENO2 + HO$_2$ → NPHENOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46437b | TrGAroCN | NPHENO2 + HO$_2$ → MALDALCO2H + GLYOX + NO$_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46438 | TrGAroCN | NPHENO2 + NO → MALDALCO2H + GLYOX + NO$_2$ + NO$_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46439 | TrGAroCN | NPHENO2 + NO$_3$ → MALDALCO2H + GLYOX + NO$_2$ + NO$_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46440 | TrGAroCN | NPHENO2 → MALDALCO2H + GLYOX + NO$_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46441 | TrGAroC | BENZENE + OH → .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO$_2$ + .53 PHENOL + .53 HO$_2$ | 2.3E-12*EXP(-190./temp) | Rickard and Pascoe (2009)* |
| G46442 | TrGAroCN | C5CO2OHPAN + OH → HOCOC4DIAL + CO + CO + NO$_2$ | 7.66E-11 | Rickard and Pascoe (2009) |
| G46443 | TrGAroCN | C5CO2OHPAN → C5CO2OHCO3 + NO$_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G46444 | TrGAroCN | CATEC1O + NO$_2$ → NCATECHOL | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G46445 | TrGAroC | CATEC1O + O$_3$ → CATEC1O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G46446 | TrGAroC | BZEMUCCO + OH → EPXDLCO3 + GLYOX | 9.20E-11 | Rickard and Pascoe (2009) |
| G46447a | TrGAroCN | NNCATECO2 + HO$_2$ → NNCATECOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46447b | TrGAroCN | NNCATECO2 + HO$_2$ → NC4DCO2H + HCOCO$_2$H + NO$_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46448 | TrGAroCN | NNCATECO2 + NO → NC4DCO2H + HCOCO$_2$H + NO$_2$ + NO$_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46449 | TrGAroCN | NNCATECO2 + NO$_3$ → NC4DCO2H + HCOCO$_2$H + NO$_2$ + NO$_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46450 | TrGAroCN | NNCATECO2 → NC4DCO2H + HCOCO$_2$H + NO$_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46451 | TrGAroC | BZEMUCCO2H + OH → C5DIALO2 + CO$_2$ | 4.06E-11 | Rickard and Pascoe (2009) |
| G46452 | TrGAroCN | NNCATECOOH + OH → NNCATECO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G46453 | TrGAroCN | NPHEN1O + NO$_2$ → DNPHEN | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46454 | TrGAroCN | NPHEN1O + $O_3$ → NPHEN1O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G46455 | TrGAroCN | DNPHEN + $NO_3$ → NDNPHENO2 | 2.25E-15 | Rickard and Pascoe (2009) |
| G46456 | TrGAroCN | DNPHEN + OH → DNPHENO2 | 3.00E-14 | Rickard and Pascoe (2009) |
| G46457 | TrGAroCN | PHENOL + $NO_3$ → .742 C6H5O + .742 $HNO_3$ + .258 NPHENO2 | 3.8E-12 | Rickard and Pascoe (2009)* |
| G46458 | TrGAroC | PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 $HO_2$ + .14 PHENO2 | 4.7E-13*EXP(1220./temp) | Rickard and Pascoe (2009)* |
| G46459 | TrGAroCN | PBZQONE + $NO_3$ → NBZQO2 | 3.00E-13 | Rickard and Pascoe (2009) |
| G46460 | TrGAroC | PBZQONE + OH → PBZQO2 | 4.6E-12 | Rickard and Pascoe (2009) |
| G46461a | TrGAroC | PHENO2 + $HO_2$ → PHENOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46461b | TrGAroC | PHENO2 + $HO_2$ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + $HO_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46462 | TrGAroCN | PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46463 | TrGAroCN | PHENO2 + $NO_3$ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46464 | TrGAroC | PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + $HO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46465 | TrGAroC | C615CO2OOH + OH → C6125CO + OH | 9.42E-11 | Rickard and Pascoe (2009) |
| G46466a | TrGAroC | C5CO2DBCO3 + $HO_2$ → C5CO2DCO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G46466b | TrGAroC | C5CO2DBCO3 + $HO_2$ → $CH_3C(O)$ + HCOCOCHO + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G46467 | TrGAroCN | C5CO2DBCO3 + NO → $CH_3C(O)$ + HCOCOCHO + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G46468 | TrGAroCN | C5CO2DBCO3 + $NO_2$ → C5CO2DBPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G46469 | TrGAroCN | C5CO2DBCO3 + $NO_3$ → $CH_3C(O)$ + HCOCOCHO + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G46470 | TrGAroC | C5CO2DBCO3 → $CH_3C(O)$ + HCOCOCHO + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G46471 | TrGAroCN | NPHEN1O2 + $HO_2$ → NPHEN1OOH | k_RO2_HO2(temp,6) | Rickard and Pascoe (2009) |
| G46472a | TrGAroCN | NPHEN1O2 + NO → NPHEN1O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G46472b | TrGAroCN | NPHEN1O2 + $NO_2$ → NPHEN1O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G46473 | TrGAroCN | NPHEN1O2 + $NO_3$ → NPHEN1O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G46474 | TrGAroCN | NPHEN1O2 → NPHEN1O | k1_RO2sRO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46475 | TrGAroCN | NPHENOOH + OH → NPHENO2 | 1.07E-10 | Rickard and Pascoe (2009) |
| G46476 | TrGAroCN | C6H5O + $NO_2$ → HOC6H4NO2 | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998)* |
| G46477 | TrGAroC | C6H5O + $O_3$ → C6H5O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G46478 | TrGAroCN | NCATECOOH + OH → NCATECO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G46479 | TrGAroC | PBZQOOH + OH → PBZQCO + OH | 1.23E-10 | Rickard and Pascoe (2009) |
| G46480a | TrGAroC | PBZQO2 + $HO_2$ → PBZQOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G46480b | TrGAroC | PBZQO2 + $HO_2$ → C5CO2OHCO3 + OH | k_RO2_HO2(temp,6)*(r_CHOHCH2O2_OH+r_COCH2O2_OH) | Rickard and Pascoe (2009)* |
| G46481 | TrGAroCN | PBZQO2 + NO → C5CO2OHCO3 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46482 | TrGAroCN | PBZQO2 + $NO_3$ → C5CO2OHCO3 + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46483 | TrGAroC | PBZQO2 → C5CO2OHCO3 | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G46484 | TrGAroC | BZOBIPEROH + OH → MALDIALCO3 + GLYOX | 8.16E-11 | Rickard and Pascoe (2009) |
| G46485a | TrGAroCN | DNPHENO2 + $HO_2$ → DNPHENOOH | k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G46485b | TrGAroCN | DNPHENO2 + $HO_2$ → NC4DCO2H + $HCOCO_2H$ + $NO_2$ + OH | k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G46486 | TrGAroCN | DNPHENO2 + NO → NC4DCO2H + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46487 | TrGAroCN | DNPHENO2 + $NO_3$ → NC4DCO2H + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46488 | TrGAroCN | DNPHENO2 → NC4DCO2H + $HCOCO_2H$ + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G46489 | TrGAroC | BZBIPEROOH + OH → BZOBIPEROH + OH | 9.77E-11 | Rickard and Pascoe (2009) |
| G46490a | TrGAroC | BZEMUCO2 + $HO_2$ → BZEMUCOOH | k_RO2_HO2(temp,6) | Rickard and Pascoe (2009) |
| G46490b | TrGAroC | BZEMUCO2 + $HO_2$ → .5 EPXC4DIAL + .5 GLYOX + .5 $HO_2$ + .5 C3DIALO2 + .5 C32OH13CO + OH | k_RO2_HO2(temp,6) | Rickard and Pascoe (2009)* |
| G46491a | TrGAroCN | BZEMUCO2 + NO → BZEMUCNO3 | KRO2NO*alpha_AN(10,2,0,1,0,temp,cair) | Rickard and Pascoe (2009) |
| G46491b | TrGAroCN | BZEMUCO2 + NO → .5 EPXC4DIAL + .5 GLYOX + .5 $HO_2$ + .5 C3DIALO2 + .5 C32OH13CO + $NO_2$ | KRO2NO*(1.-alpha_AN(10,2,0,1,0,temp,cair)) | Rickard and Pascoe (2009)* |
| G46492 | TrGAroCN | BZEMUCO2 + $NO_3$ → .5 EPXC4DIAL + .5 GLYOX + .5 $HO_2$ + .5 C3DIALO2 + .5 C32OH13CO + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46493 | TrGAroC | BZEMUCO2 $\rightarrow$ .5 EPXC4DIAL + .5 GLYOX + .5 $HO_2$ + .5 C3DIALO2 + .5 C32OH13CO | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G46494 | TrGAroCN | C5CO2DBPAN + OH $\rightarrow$ HCOCOCHO + $CH_3CHO$ + $CO_2$ + $NO_2$ | 3.28E-11 | Rickard and Pascoe (2009) |
| G46495 | TrGAroCN | C5CO2DBPAN $\rightarrow$ C5CO2DBCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G46496 | TrGAroCN | NBZQOOH + OH $\rightarrow$ NBZQO2 | 6.68E-11 | Rickard and Pascoe (2009) |
| G46497 | TrGAroC | CATEC1OOH + OH $\rightarrow$ CATEC1O2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G46498 | TrGAroC | C6125CO + OH $\rightarrow$ C5CO14O2 + CO | 6.45E-11 | Rickard and Pascoe (2009) |
| G46499a | TrGAroCN | NBZQO2 + $HO_2$ $\rightarrow$ NBZQOOH | k_RO2_HO2(temp,6)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G46499b | TrGAroCN | NBZQO2 + $HO_2$ $\rightarrow$ C6CO4DB + $NO_2$ + OH | k_RO2_HO2(temp,6)*r_COCH2O2_OH | Rickard and Pascoe (2009)* |
| G46500 | TrGAroCN | NBZQO2 + NO $\rightarrow$ C6CO4DB + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G46501 | TrGAroCN | NBZQO2 + $NO_3$ $\rightarrow$ C6CO4DB + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46502 | TrGAroCN | NBZQO2 $\rightarrow$ C6CO4DB + $NO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G46503 | TrGAroCN | DNPHENOOH + OH $\rightarrow$ DNPHENO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G46504 | TrGAroC | CATEC1O2 + $HO_2$ $\rightarrow$ CATEC1OOH | k_RO2_HO2(temp,6) | Rickard and Pascoe (2009) |
| G46505a | TrGAroCN | CATEC1O2 + NO $\rightarrow$ CATEC1O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G46505b | TrGAroCN | CATEC1O2 + $NO_2$ $\rightarrow$ CATEC1O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G46506 | TrGAroCN | CATEC1O2 + $NO_3$ $\rightarrow$ CATEC1O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G46507 | TrGAroC | CATEC1O2 $\rightarrow$ CATEC1O | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G46508 | TrGAroC | BZEMUCCO3H + OH $\rightarrow$ BZEMUCCO3 | 4.37E-11 | Rickard and Pascoe (2009) |
| G46509 | TrGAroC | C6H5OOH + OH $\rightarrow$ C6H5O2 | 3.60E-12 | Rickard and Pascoe (2009) |
| G46510 | TrGAroC | BZEMUCOOH + OH $\rightarrow$ BZEMUCCO + OH | 1.31E-10 | Rickard and Pascoe (2009) |
| G46511a | TrGAroC | BZEMUCCO3 + $HO_2$ $\rightarrow$ BZEMUCCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G46511b | TrGAroC | BZEMUCCO3 + $HO_2$ $\rightarrow$ BZEMUCCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G46511c | TrGAroC | BZEMUCCO3 + $HO_2$ $\rightarrow$ C5DIALO2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G46512 | TrGAroCN | BZEMUCCO3 + NO $\rightarrow$ C5DIALO2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G46513 | TrGAroCN | BZEMUCCO3 + $NO_2$ $\rightarrow$ BZEMUCPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G46514 | TrGAroCN | BZEMUCCO3 + $NO_3$ $\rightarrow$ C5DIALO2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G46515 | TrGAroC | BZEMUCCO3 $\rightarrow$ C5DIALO2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G46516 | TrGAroC | C6H5O2 + $HO_2$ $\rightarrow$ C6H5OOH | k_RO2_HO2(temp,6) | Rickard and Pascoe (2009) |
| G46517 | TrGAroCN | C6H5O2 + NO $\rightarrow$ C6H5O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G46518 | TrGAroCN | C6H5O2 + $NO_3$ $\rightarrow$ C6H5O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G46519 | TrGAroC | C6H5O2 $\rightarrow$ C6H5O | k1_RO2sRO2 | Rickard and Pascoe (2009) |
| G46520 | TrGAroCN | C6H5O2 + $NO_2$ $\rightarrow$ C6H5O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G46521 | TrGAroCN | BZEMUCNO3 + OH → BZEMUCCO + $NO_2$ | 4.38E-11 | Rickard and Pascoe (2009) |
| G46522a | TrGAroC | BZBIPERO2 + $HO_2$ → BZBIPEROOH | k_RO2_HO2(temp,6)*(1.-r_BIPERO2_OH) | Rickard and Pascoe (2009) |
| G46522b | TrGAroC | BZBIPERO2 + $HO_2$ → OH + GLYOX + $HO_2$ + .5 BZFUONE + .5 BZFUONE | k_RO2_HO2(temp,6)*r_BIPERO2_OH | Rickard and Pascoe (2009), Birdsall et al. (2010)* |
| G46523a | TrGAroCN | BZBIPERO2 + NO → BZBIPERNO3 | KRO2NO*alpha_AN(9,2,0,0,1,temp,cair) | Rickard and Pascoe (2009) |
| G46523b | TrGAroCN | BZBIPERO2 + NO → $NO_2$ + GLYOX + $HO_2$ + .5 BZFUONE + .5 BZFUONE | KRO2NO*(1.-alpha_AN(9,2,0,0,1,temp,cair)) | Rickard and Pascoe (2009)* |
| G46524 | TrGAroCN | BZBIPERO2 + $NO_3$ → $NO_2$ + GLYOX + $HO_2$ + .5 BZFUONE + .5 BZFUONE | KRO2NO3 | Rickard and Pascoe (2009)* |
| G46525 | TrGAroC | BZBIPERO2 → GLYOX + $HO_2$ + BZFUONE | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G47200 | TrGTerCN | CO235C6CHO + $NO_3$ → CO235C6CO3 + $HNO_3$ | KNO3AL*5.5 | Rickard and Pascoe (2009) |
| G47201 | TrGTerC | CO235C6CHO + OH → CO235C6CO3 | 6.70E-11 | Rickard and Pascoe (2009) |
| G47202a | TrGTerC | CO235C6CO3 + $HO_2$ → C235C6CO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G47202b | TrGTerC | CO235C6CO3 + $HO_2$ → CO235C6O2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G47203 | TrGTerCN | CO235C6CO3 + NO → CO235C6O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47204 | TrGTerCN | CO235C6CO3 + $NO_2$ → C7PAN3 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G47205 | TrGTerC | CO235C6CO3 → CO235C6O2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G47206 | TrGTerC | C235C6CO3H + OH → CO235C6CO3 | 4.75E-12 | Rickard and Pascoe (2009) |
| G47207 | TrGTerCN | C7PAN3 + OH → CO235C5CHO + CO + $NO_2$ | 8.83E-13 | Rickard and Pascoe (2009) |
| G47208 | TrGTerCN | C7PAN3 → CO235C6CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G47209a | TrGTerC | C716O2 + $HO_2$ → C716OOH | k_RO2_HO2(temp,7)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G47209b | TrGTerC | C716O2 + $HO_2$ → CO13C4CHO + $CH_3C(O)$ + OH | k_RO2_HO2(temp,7)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G47210 | TrGTerCN | C716O2 + NO → CO13C4CHO + $CH_3C(O)$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47211 | TrGTerC | C716O2 → CO13C4CHO + $CH_3C(O)$ | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G47212 | TrGTerC | C716OOH + OH → CO235C6CHO + OH | 1.20E-10 | Rickard and Pascoe (2009) |
| G47213 | TrGTerC | C721O2 + $HO_2$ → C721OOH | k_RO2_HO2(temp,7) | Rickard and Pascoe (2009) |
| G47214 | TrGTerCN | C721O2 + NO → C722O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47215 | TrGTerC | C721O2 → C722O2 | k1_RO2pRO2 | Rickard and Pascoe (2009) |
| G47216 | TrGTerC | C721OOH + OH → C721O2 | 1.27E-11 | Rickard and Pascoe (2009) |
| G47217 | TrGTerC | C722O2 + $HO_2$ → C722OOH | k_RO2_HO2(temp,7) | Rickard and Pascoe (2009) |
| G47218 | TrGTerCN | C722O2 + NO → $CH_3COCH_3$ + C44O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47219 | TrGTerC | C722O2 → $CH_3COCH_3$ + C44O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G47220 | TrGTerC | C722OOH + OH → C722O2 | 3.31E-11 | Rickard and Pascoe (2009) |
| G47221 | TrGTerC | ROO6R3O2 → ROO6R5O2 | 5.68E10*EXP(-8745./temp) | Vereecken and Peeters (2012) |
| G47222 | TrGTerCN | ROO6R3O2 + NO → ROO6R3O + $NO_2$ | KRO2NO | Vereecken and Peeters (2012)* |
| G47223 | TrGTerC | ROO6R3O2 + $HO_2$ → 7 LCARBON | k_RO2_HO2(temp,7) | Vereecken and Peeters (2012)* |
| G47224 | TrGTerC | ROO6R3O2 → ROO6R3O | k1_RO2sRO2 | Vereecken and Peeters (2012) |
| G47225 | TrGTerC | ROO6R3O → 7 LCARBON + $HO_2$ | 5.7E10*EXP(-2949./temp) | Vereecken and Peeters (2012)* |
| G47226 | TrGTerC | ROO6R5O2 → 7 LCARBON + OH | 9.17E10*EXP(-8706./temp) | Vereecken and Peeters (2012)* |
| G47400 | TrGAroC | TOLUENE + OH → .07 C6H5CH2O2 + .18 CRESOL + .18 $HO_2$ + .65 TLBIPERO2 + .10 TLEPOXMUC + .10 $HO_2$ | 1.8E-12*EXP(340./temp) | Rickard and Pascoe (2009)* |
| G47401 | TrGAroC | C6H5CH2O2 + $HO_2$ → C6H5CH2OOH | 1.5E-13*EXP(1310./temp) | Rickard and Pascoe (2009) |
| G47402a | TrGAroCN | C6H5CH2O2 + NO → C6H5CH2NO3 | KRO2NO*alpha_AN(7,1,0,0,0,temp, cair) | Rickard and Pascoe (2009)* |
| G47402b | TrGAroCN | C6H5CH2O2 + NO → BENZAL + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(7,1,0,0,0, temp,cair)) | Rickard and Pascoe (2009)* |
| G47403 | TrGAroCN | C6H5CH2O2 + $NO_3$ → BENZAL + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47404 | TrGAroC | C6H5CH2O2 → BENZAL + $HO_2$ | 2.*(k_CH3O2*2.4E-14*EXP(1620./ temp))**(0.5)*RO2 | Rickard and Pascoe (2009)* |
| G47405 | TrGAroCN | CRESOL + $NO_3$ → .103 CRESO2 + .103 $HNO_3$ + .506 NCRESO2 + .391 TOL1O + .391 $HNO_3$ | 1.4E-11 | Rickard and Pascoe (2009)* |
| G47406 | TrGAroC | CRESOL + OH → .2 CRESO2 + .727 MCATECHOL + .727 $HO_2$ + .073 TOL1O | 4.65E-11 | Rickard and Pascoe (2009)* |
| G47407a | TrGAroC | TLBIPERO2 + $HO_2$ → TLBIPEROOH | k_RO2_HO2(temp,7)*(1.-r_BIPERO2_ OH) | Rickard and Pascoe (2009) |
| G47407b | TrGAroC | TLBIPERO2 + $HO_2$ → OH + .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | k_RO2_HO2(temp,7)*r_BIPERO2_OH | Rickard and Pascoe (2009), Birdsall et al. (2010)* |
| G47408a | TrGAroCN | TLBIPERO2 + NO → $NO_2$ + .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | KRO2NO*(1.-alpha_AN(11,2,0,0,1, temp,cair)) | Rickard and Pascoe (2009)* |
| G47408b | TrGAroCN | TLBIPERO2 + NO → TLBIPERNO3 | KRO2NO*alpha_AN(11,2,0,0,1, temp,cair) | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47409 | TrGAroCN | TLBIPERO2 + $NO_3$ → $NO_2$ + .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47410 | TrGAroC | TLBIPERO2 → .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G47411 | TrGAroCN | TLEPOXMUC + $NO_3$ → TLEMUCCO3 + $HNO_3$ | KNO3AL*2.75 | Rickard and Pascoe (2009) |
| G47412 | TrGAroC | TLEPOXMUC + $O_3$ → EPXC4DIAL + .125 $CH_3CHO$ + .695 $CH_3C(O)$ + .57 CO + .57 OH + .125 $HO_2$ + .1125 $CH_3COCO_2H$ + .0675 MGLYOX + .0675 $H_2O_2$ + .25 $CO_2$ | 5.00E-18 | Rickard and Pascoe (2009)* |
| G47413 | TrGAroC | TLEPOXMUC + OH → .31 TLEMUCCO3 + .69 TLEMUCO2 | 7.99E-11 | Rickard and Pascoe (2009)* |
| G47414 | TrGAroC | C6H5CH2OOH + OH → BENZAL + OH | 2.05E-11 | Rickard and Pascoe (2009) |
| G47415 | TrGAroCN | C6H5CH2NO3 + OH → BENZAL + $NO_2$ | 6.03E-12 | Rickard and Pascoe (2009) |
| G47416 | TrGAroCN | BENZAL + $NO_3$ → C6H5CO3 + $HNO_3$ | 2.40E-15 | Rickard and Pascoe (2009) |
| G47417 | TrGAroC | BENZAL + OH → C6H5CO3 | 5.9E-12*EXP(225./temp) | Rickard and Pascoe (2009) |
| G47418a | TrGAroC | CRESO2 + $HO_2$ → CRESOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47418b | TrGAroC | CRESO2 + $HO_2$ → .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47419 | TrGAroCN | CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47420 | TrGAroCN | CRESO2 + $NO_3$ → .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47421 | TrGAroC | CRESO2 → .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G47422a | TrGAroCN | NCRESO2 + $HO_2$ → NCRESOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47422b | TrGAroCN | NCRESO2 + $HO_2$ → C5CO14OH + GLYOX + $NO_2$ + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47423 | TrGAroCN | NCRESO2 + NO → C5CO14OH + GLYOX + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47424 | TrGAroCN | NCRESO2 + $NO_3$ → C5CO14OH + GLYOX + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47425 | TrGAroCN | NCRESO2 → C5CO14OH + GLYOX + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47426 | TrGAroCN | TOL1O + $NO_2$ → TOL1OHNO2 | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998)* |
| G47427 | TrGAroC | TOL1O + $O_3$ → OXYL1O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G47428 | TrGAroCN | MCATECHOL + $NO_3$ → MCATEC1O + $HNO_3$ | 1.7E-10*1.0 | Rickard and Pascoe (2009) |
| G47429 | TrGAroC | MCATECHOL + $O_3$ → MC3ODBCO2H + $HCOCO_2H$ + $HO_2$ + OH | 2.8E-17 | Rickard and Pascoe (2009)* |
| G47430 | TrGAroC | MCATECHOL + OH → MCATEC1O | 2.0E-10*1.0 | Rickard and Pascoe (2009) |
| G47431 | TrGAroC | TLBIPEROOH + OH → TLOBIPEROH + OH | 9.64E-11 | Rickard and Pascoe (2009) |
| G47432 | TrGAroCN | TLBIPERNO3 + OH → TLOBIPEROH + $NO_2$ | 7.16E-11 | Rickard and Pascoe (2009) |
| G47433 | TrGAroC | TLOBIPEROH + OH → C5CO14O2 + GLYOX | 7.99E-11 | Rickard and Pascoe (2009) |
| G47434a | TrGAroC | TLEMUCCO3 + $HO_2$ → C615CO2O2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G47434b | TrGAroC | TLEMUCCO3 + $HO_2$ → TLEMUCCO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G47434c | TrGAroC | TLEMUCCO3 + $HO_2$ → TLEMUCCO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G47435 | TrGAroCN | TLEMUCCO3 + NO → C615CO2O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47436 | TrGAroCN | TLEMUCCO3 + $NO_2$ → TLEMUCPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G47437 | TrGAroCN | TLEMUCCO3 + $NO_3$ → C615CO2O2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G47438 | TrGAroC | TLEMUCCO3 → C615CO2O2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G47439a | TrGAroC | TLEMUCO2 + $HO_2$ → TLEMUCOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G47439b | TrGAroC | TLEMUCO2 + $HO_2$ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 $HO_2$ + OH | k_RO2_HO2(temp,7)*(r_CHOHCH2O2_OH+r_COCH2O2_OH) | Rickard and Pascoe (2009)* |
| G47440a | TrGAroCN | TLEMUCO2 + NO → TLEMUCNO3 | KRO2NO*alpha_AN(11,2,1,0,0, temp,cair) | Rickard and Pascoe (2009) |
| G47440b | TrGAroCN | TLEMUCO2 + NO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(11,2,1,0,0, temp,cair)) | Rickard and Pascoe (2009)* |
| G47441 | TrGAroCN | TLEMUCO2 + $NO_3$ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47442 | TrGAroC | TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 $HO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G47443a | TrGAroC | C6H5CO3 + $HO_2$ → C6H5CO3H | 1.1E-11*EXP(364./temp)*0.65 | Roth et al. (2010) |
| G47443b | TrGAroC | C6H5CO3 + $HO_2$ → C6H5O2 + $CO_2$ + OH | 1.1E-11*EXP(364./temp)*0.20 | Roth et al. (2010) |
| G47443c | TrGAroC | C6H5CO3 + $HO_2$ → PHCOOH + $O_3$ | 1.1E-11*EXP(364./temp)*0.15 | Roth et al. (2010) |
| G47444 | TrGAroCN | C6H5CO3 + NO → C6H5O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47445 | TrGAroCN | C6H5CO3 + $NO_2$ → PBZN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47446 | TrGAroCN | C6H5CO3 + $NO_3$ → C6H5O2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G47447 | TrGAroC | C6H5CO3 → C6H5O2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009)* |
| G47448 | TrGAroC | CRESOOH + OH → CRESO2 | 1.15E-10 | Rickard and Pascoe (2009) |
| G47449 | TrGAroCN | NCRESOOH + OH → NCRESO2 | 1.07E-10 | Rickard and Pascoe (2009) |
| G47450 | TrGAroCN | TOL1OHNO2 + $NO_3$ → NCRES1O + $HNO_3$ | 3.13E-13*1.0 | Rickard and Pascoe (2009) |
| G47451 | TrGAroCN | TOL1OHNO2 + OH → NCRES1O | 2.8E-12 | Rickard and Pascoe (2009) |
| G47452 | TrGAroC | OXYL1O2 + $HO_2$ → OXYL1OOH | k_RO2_HO2(temp,7) | Rickard and Pascoe (2009) |
| G47453 | TrGAroCN | OXYL1O2 + NO → TOL1O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G47454 | TrGAroCN | OXYL1O2 + $NO_2$ → TOL1O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G47455 | TrGAroCN | OXYL1O2 + $NO_3$ → TOL1O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G47456 | TrGAroC | OXYL1O2 → TOL1O | k1_RO2sRO2 | Rickard and Pascoe (2009) |
| G47457 | TrGAroCN | MCATEC1O + $NO_2$ → MNCATECH | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G47458 | TrGAroC | MCATEC1O + $O_3$ → MCATEC1O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G47459 | TrGAroC | TLEMUCCO2H + OH → C615CO2O2 + $CO_2$ | 5.98E-11 | Rickard and Pascoe (2009) |
| G47460 | TrGAroC | TLEMUCCO3H + OH → TLEMUCCO3 | 6.29E-11 | Rickard and Pascoe (2009) |
| G47461 | TrGAroCN | TLEMUCPAN + OH → C5DICARB + CO + $CO_2$ + $NO_2$ | 5.96E-11 | Rickard and Pascoe (2009) |
| G47462 | TrGAroCN | TLEMUCPAN → TLEMUCCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G47463 | TrGAroC | TLEMUCOOH + OH → TLEMUCCO + OH | 7.04E-11 | Rickard and Pascoe (2009) |
| G47464 | TrGAroCN | TLEMUCNO3 + OH → TLEMUCCO + $NO_2$ | 3.06E-11 | Rickard and Pascoe (2009) |
| G47465 | TrGAroC | TLEMUCCO + OH → $CH_3C(O)$ + EPXC4DIAL + CO | 4.06E-11 | Rickard and Pascoe (2009) |
| G47466 | TrGAroC | C6H5CO3H + OH → C6H5CO3 | 4.66E-12 | Rickard and Pascoe (2009) |
| G47467 | TrGAroC | PHCOOH + OH → C6H5O2 + $CO_2$ | 1.10E-12 | Rickard and Pascoe (2009) |
| G47468 | TrGAroCN | PBZN + OH → C6H5OOH + CO + $NO_2$ | 1.06E-12 | Rickard and Pascoe (2009) |
| G47469 | TrGAroCN | PBZN → C6H5CO3 + $NO_2$ | k_PAN_M*0.67 | Rickard and Pascoe (2009) |
| G47470 | TrGAroCN | PTLQONE + $NO_3$ → NPTLQO2 | 1.00E-12 | Rickard and Pascoe (2009) |
| G47471 | TrGAroC | PTLQONE + OH → PTLQO2 | 2.3E-11 | Rickard and Pascoe (2009) |
| G47472 | TrGAroCN | NCRES1O + $NO_2$ → DNCRES | k_C6H5O_NO2 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G47473 | TrGAroCN | NCRES1O + $O_3$ → NCRES1O2 | k_C6H5O_O3 | Rickard and Pascoe (2009), Tao and Li (1999) |
| G47474 | TrGAroC | OXYL1OOH + OH → OXYL1O2 | 4.65E-11 | Rickard and Pascoe (2009) |
| G47475 | TrGAroCN | MNCATECH + $NO_3$ → MNNCATECO2 | 5.03E-12 | Rickard and Pascoe (2009) |
| G47476 | TrGAroCN | MNCATECH + OH → MNCATECO2 | 6.83E-12 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47477 | TrGAroC | MCATEC1O2 + $HO_2$ → MCATEC1OOH | k_RO2_HO2(temp,7) | Rickard and Pascoe (2009) |
| G47478 | TrGAroCN | MCATEC1O2 + NO → MCATEC1O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G47479 | TrGAroCN | MCATEC1O2 + $NO_2$ → MCATEC1O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G47480 | TrGAroCN | MCATEC1O2 + $NO_3$ → MCATEC1O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G47481 | TrGAroC | MCATEC1O2 → MCATEC1O | k1_RO2sORO2 | Rickard and Pascoe (2009) |
| G47482a | TrGAroCN | NPTLQO2 + $HO_2$ → NPTLQOOH | k_RO2_HO2(temp,7)*(1.-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G47482b | TrGAroCN | NPTLQO2 + $HO_2$ → C7CO4DB + $NO_2$ + OH | k_RO2_HO2(temp,7)*r_COCH2O2_OH | Rickard and Pascoe (2009)* |
| G47483 | TrGAroCN | NPTLQO2 + NO → C7CO4DB + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47484 | TrGAroCN | NPTLQO2 + $NO_3$ → C7CO4DB + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47485 | TrGAroCN | NPTLQO2 → C7CO4DB + $NO_2$ | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G47486a | TrGAroC | PTLQO2 + $HO_2$ → PTLQOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH) | Rickard and Pascoe (2009) |
| G47486b | TrGAroC | PTLQO2 + $HO_2$ → C6CO2OHCO3 + OH | k_RO2_HO2(temp,7)*(r_CHOHCH2O2_OH+r_COCH2O2_OH) | Rickard and Pascoe (2009)* |
| G47487 | TrGAroCN | PTLQO2 + NO → C6CO2OHCO3 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47488 | TrGAroCN | PTLQO2 + $NO_3$ → C6CO2OHCO3 + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47489 | TrGAroC | PTLQO2 → C6CO2OHCO3 | k1_RO2sORO2 | Rickard and Pascoe (2009)* |
| G47490 | TrGAroCN | DNCRES + $NO_3$ → NDNCRESO2 | 7.83E-15 | Rickard and Pascoe (2009) |
| G47491 | TrGAroCN | DNCRES + OH → DNCRESO2 | 5.10E-14 | Rickard and Pascoe (2009) |
| G47492 | TrGAroCN | NCRES1O2 + $HO_2$ → NCRES1OOH | k_RO2_HO2(temp,7) | Rickard and Pascoe (2009) |
| G47493 | TrGAroCN | NCRES1O2 + NO → NCRES1O + $NO_2$ | KRO2NO | Rickard and Pascoe (2009) |
| G47494 | TrGAroCN | NCRES1O2 + $NO_2$ → NCRES1O + $NO_3$ | k_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G47495 | TrGAroCN | NCRES1O2 + $NO_3$ → NCRES1O + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G47496 | TrGAroCN | NCRES1O2 → NCRES1O | k1_RO2sRO2 | Rickard and Pascoe (2009) |
| G47497a | TrGAroCN | MNNCATECO2 + $HO_2$ → MNNCATCOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47497b | TrGAroCN | MNNCATECO2 + $HO_2$ → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47498 | TrGAroCN | MNNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47499 | TrGAroCN | MNNCATECO2 + $NO_3$ → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47500 | TrGAroCN | MNNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47501a | TrGAroCN | MNCATECO2 + $HO_2$ → MNCATECOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47501b | TrGAroCN | MNCATECO2 + $HO_2$ → NC4MDCO2HN + $HCOCO_2H$ + $HO_2$ + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47502 | TrGAroCN | MNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + $HO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47503 | TrGAroCN | MNCATECO2 + $NO_3$ → NC4MDCO2HN + $HCOCO_2H$ + $HO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47504 | TrGAroCN | MNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + $HO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G47505 | TrGAroC | MCATEC1OOH + OH → MCATEC1O2 | 2.05E-10 | Rickard and Pascoe (2009) |
| G47506 | TrGAroCN | NPTLQOOH + OH → NPTLQO2 | 8.56E-11 | Rickard and Pascoe (2009) |
| G47507 | TrGAroC | PTLQOOH + OH → PTLQCO + OH | 1.42E-10 | Rickard and Pascoe (2009) |
| G47508 | TrGAroC | PTLQCO + OH → C6CO2OHCO3 | 7.95E-11 | Rickard and Pascoe (2009) |
| G47509a | TrGAroCN | NDNCRESO2 + $HO_2$ → NDNCRESOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47509b | TrGAroCN | NDNCRESO2 + $HO_2$ → NC4MDCO2HN + $HNO_3$ + 2 CO + $NO_2$ + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47510 | TrGAroCN | NDNCRESO2 + NO → NC4MDCO2HN + $HNO_3$ + 2 CO + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47511 | TrGAroCN | NDNCRESO2 + $NO_3$ → NC4MDCO2HN + $HNO_3$ + 2 CO + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47512 | TrGAroCN | NDNCRESO2 → NC4MDCO2HN + $HNO_3$ + 2 CO + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G47513a | TrGAroCN | DNCRESO2 + $HO_2$ → DNCRESOOH | k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G47513b | TrGAroCN | DNCRESO2 + $HO_2$ → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + OH | k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G47514 | TrGAroCN | DNCRESO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G47515 | TrGAroCN | DNCRESO2 + $NO_3$ → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009)* |
| G47516 | TrGAroCN | DNCRESO2 → NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ | k1_RO2ISOPDO2 | Rickard and Pascoe (2009)* |
| G47517 | TrGAroCN | NCRES1OOH + OH → NCRES1O2 | 1.53E-12 | Rickard and Pascoe (2009) |
| G47518 | TrGAroCN | MNNCATCOOH + OH → MNNCATECO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G47519 | TrGAroCN | MNCATECOOH + OH → MNCATECO2 | k_ROOHRO | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G47520 | TrGAroC | C7CO4DB + OH → CO + CO + $CH_3C(O)$ + HCOCOCHO | 9.58E-11 | Rickard and Pascoe (2009) |
| G47521a | TrGAroC | C6CO2OHCO3 + $HO_2$ → C5134CO2OH + $HO_2$ + CO + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G47521b | TrGAroC | C6CO2OHCO3 + $HO_2$ → C6COOHCO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G47522 | TrGAroCN | C6CO2OHCO3 + NO → C5134CO2OH + $HO_2$ + CO + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47523 | TrGAroCN | C6CO2OHCO3 + $NO_2$ → C6CO2OHPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G47524 | TrGAroCN | C6CO2OHCO3 + $NO_3$ → C5134CO2OH + $HO_2$ + CO + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G47525 | TrGAroC | C6CO2OHCO3 → C5134CO2OH + $HO_2$ + CO + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G47526 | TrGAroCN | NDNCRESOOH + OH → NDNCRESO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G47527 | TrGAroCN | DNCRESOOH + OH → DNCRESO2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G47528 | TrGAroC | C6COOHCO3H + OH → C6CO2OHCO3 | 9.29E-11 | Rickard and Pascoe (2009) |
| G47529 | TrGAroCN | C6CO2OHPAN + OH → C5134CO2OH + CO + CO + $NO_2$ | 8.96E-11 | Rickard and Pascoe (2009) |
| G47530 | TrGAroCN | C6CO2OHPAN → C6CO2OHCO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G48200 | TrGTerC | C85O2 → C86O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G48201 | TrGTerC | C85O2 + $HO_2$ → C85OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48202 | TrGTerCN | C85O2 + NO → C86O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G48203 | TrGTerC | C85OOH + OH → C85O2 | 1.29E-11 | Rickard and Pascoe (2009) |
| G48204 | TrGTerC | C86O2 → C511O2 + $CH_3COCH_3$ | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G48205 | TrGTerCN | C86O2 + NO → C511O2 + $CH_3COCH_3$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G48206 | TrGTerC | C86O2 + $HO_2$ → C86OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48207 | TrGTerC | C86OOH + OH → C86O2 | 3.45E-11 | Rickard and Pascoe (2009) |
| G48208 | TrGTerC | C811O2 → C812O2 | k1_RO2pRO2 | Rickard and Pascoe (2009) |
| G48209 | TrGTerC | C811O2 + $HO_2$ → 8 LCARBON | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48210 | TrGTerCN | C811O2 + NO → C812O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G48211 | TrGTerC | C812O2 → C813O2 | k1_RO2tORO2 | Rickard and Pascoe (2009) |
| G48212 | TrGTerCN | C812O2 + NO → C813O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G48213 | TrGTerC | C812O2 + $HO_2$ → C812OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48214 | TrGTerC | C812OOH + OH → C812O2 | 1.09E-11 | Rickard and Pascoe (2009) |
| G48215 | TrGTerC | C813O2 → $CH_3COCH_3$ + C512O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G48216 | TrGTerCN | C813O2 + NO → $CH_3COCH_3$ + C512O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G48217 | TrGTerC | C813O2 + $HO_2$ → C813OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G48218 | TrGTerC | C813OOH + OH → C813O2 | 1.86E-11 | Rickard and Pascoe (2009) |
| G48219 | TrGTerCN | C721CHO + $NO_3$ → C721CO3 + $HNO_3$ | KNO3AL*8.5 | Rickard and Pascoe (2009) |
| G48220 | TrGTerC | C721CHO + OH → C721CO3 | 2.63E-11 | Rickard and Pascoe (2009) |
| G48221a | TrGTerC | C721CO3 + $HO_2$ → C721CO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G48221b | TrGTerC | C721CO3 + $HO_2$ → C721O2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G48221c | TrGTerC | C721CO3 + $HO_2$ → NORPINIC + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G48222 | TrGTerCN | C721CO3 + NO → C721O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G48223 | TrGTerCN | C721CO3 + $NO_2$ → C721PAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G48224 | TrGTerCN | C721CO3 + $NO_3$ → C721O2 + $CO_2$ + $NO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G48225 | TrGTerC | C721CO3 → C721O2 + $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G48226 | TrGTerC | C721CO3 → NORPINIC | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G48227 | TrGTerC | C721CO3H + OH → C721CO3 | 9.65E-12 | Rickard and Pascoe (2009) |
| G48228 | TrGTerC | NORPINIC + OH → C721O2 + $CO_2$ | 6.57E-12 | Rickard and Pascoe (2009) |
| G48229 | TrGTerCN | C721PAN + OH → C721OOH + CO + $NO_2$ | 2.96E-12 | Rickard and Pascoe (2009) |
| G48230 | TrGTerCN | C721PAN → C721CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G48231 | TrGTerC | C8BC + OH → C8BCO2 | 3.04E-12 | Rickard and Pascoe (2009) |
| G48232 | TrGTerC | C8BCO2 + $HO_2$ → C8BCOOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48233a | TrGTerCN | C8BCO2 + NO → C89O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(8,2,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G48233b | TrGTerCN | C8BCO2 + NO → C8BCNO3 | KRO2NO*alpha_AN(8,2,0,0,0,temp, cair) | Rickard and Pascoe (2009) |
| G48234 | TrGTerC | C8BCO2 → C89O2 | k1_RO2sRO2 | Rickard and Pascoe (2009) |
| G48235 | TrGTerC | C8BCOOH + OH → C8BCCO + OH | 1.62E-11 | Rickard and Pascoe (2009) |
| G48236 | TrGTerCN | C8BCNO3 + OH → C8BCCO + $NO_2$ | 1.84E-12 | Rickard and Pascoe (2009) |
| G48237 | TrGTerC | C8BCCO + OH → C89O2 | 3.94E-12 | Rickard and Pascoe (2009) |
| G48238 | TrGTerC | C89O2 + $HO_2$ → C89OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48239a | TrGTerCN | C89O2 + NO → C810O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(7,2,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G48239b | TrGTerCN | C89O2 + NO → C89NO3 | KRO2NO*alpha_AN(7,2,0,0,0,temp, cair) | Rickard and Pascoe (2009) |
| G48240 | TrGTerCN | C89O2 + $NO_3$ → C810O2 + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G48241 | TrGTerC | C89O2 → C810O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G48242 | TrGTerC | C89OOH + OH → C89O2 | 3.61E-11 | Rickard and Pascoe (2009) |
| G48243 | TrGTerCN | C89NO3 + OH → $CH_3COCH_3$ + CO13C4CHO + $NO_2$ | 2.56E-11 | Rickard and Pascoe (2009) |
| G48244 | TrGTerC | C810O2 + $HO_2$ → C810OOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G48245a | TrGTerCN | C810O2 + NO → $CH_3COCH_3$ + C514O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(10,3,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G48245b | TrGTerCN | C810O2 + NO → C810NO3 | KRO2NO*alpha_AN(10,3,0,0,0, temp,cair) | Rickard and Pascoe (2009) |
| G48246 | TrGTerCN | C810O2 + $NO_3$ → $CH_3COCH_3$ + C514O2 + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G48247 | TrGTerC | C810O2 → $CH_3COCH_3$ + C514O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G48248 | TrGTerC | C810OOH + OH → C810O2 | 8.35E-11 | Rickard and Pascoe (2009) |
| G48249 | TrGTerCN | C810NO3 + OH → $CH_3COCH_3$ + CO13C4CHO + $NO_2$ | 4.96E-11 | Rickard and Pascoe (2009) |
| G48400a | TrGAroC | LXYL + OH → TLEPOXMUC + $HO_2$ + LCARBON | 0.401E-11 | Rickard and Pascoe (2009)* |
| G48400b | TrGAroC | LXYL + OH → C6H5CH2O2 + LCARBON | 0.101E-11 | Rickard and Pascoe (2009)* |
| G48400c | TrGAroC | LXYL + OH → CRESOL + LCARBON | 0.261E-11 | Rickard and Pascoe (2009)* |
| G48400d | TrGAroC | LXYL + OH → TLBIPERO2 + $HO_2$ + LCARBON | 0.932E-11 | Rickard and Pascoe (2009)* |
| G48401 | TrGAroCN | LXYL + $NO_3$ → C6H5CH2O2 + $HNO_3$ + LCARBON | 3.9E-16 | Rickard and Pascoe (2009)* |
| G48402 | TrGAroC | EBENZ + OH → .10 TLEPOXMUC + .07 C6H5CH2O2 + .18 CRESOL + .65 TLBIPERO2 + .28 $HO_2$ + LCARBON | 7.00E-12 | Rickard and Pascoe (2009)* |
| G48403 | TrGAroCN | EBENZ + $NO_3$ → C6H5CH2O2 + $HNO_3$ + LCARBON | 1.20E-16 | Rickard and Pascoe (2009)* |
| G48404 | TrGAroCN | STYRENE + $NO_3$ → NSTYRENO2 | 1.50E-12 | Rickard and Pascoe (2009) |
| G48405 | TrGAroC | STYRENE + $O_3$ → .545 HCHO + .1 BENZENE + .28 C6H5O2 + .56 CO + .36 OH + .28 $HO_2$ + .075 PHCOOH + .545 BENZAL + .09 $H_2O_2$ + .075 HCOOH + .2 $CO_2$ | 1.70E-17 | Rickard and Pascoe (2009)* |
| G48406 | TrGAroC | STYRENE + OH → STYRENO2 | 5.80E-11 | Rickard and Pascoe (2009) |
| G48407 | TrGAroCN | NSTYRENO2 + $HO_2$ → NSTYRENOOH | k_RO2_HO2(temp,8) | Rickard and Pascoe (2009) |
| G48408 | TrGAroCN | NSTYRENO2 + NO → $NO_2$ + $NO_2$ + HCHO + BENZAL | KRO2NO | Rickard and Pascoe (2009)* |
| G48409 | TrGAroCN | NSTYRENO2 + $NO_3$ → $NO_2$ + $NO_2$ + HCHO + BENZAL | KRO2NO3 | Rickard and Pascoe (2009)* |
| G48410 | TrGAroCN | NSTYRENO2 → $NO_2$ + HCHO + BENZAL | k1_RO2sRO2 | Rickard and Pascoe (2009)* |
| G48411 | TrGAroCN | NSTYRENOOH + OH → NSTYRENO2 | 6.16E-11 | Rickard and Pascoe (2009) |
| G48412a | TrGAroC | STYRENO2 + $HO_2$ → STYRENOOH | k_RO2_HO2(temp,8)*(1.-r_ CHOHCH2O2_OH) | Rickard and Pascoe (2009) |
| G48412b | TrGAroC | STYRENO2 + $HO_2$ → $HO_2$ + OH + HCHO + BENZAL | k_RO2_HO2(temp,8)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009)* |
| G48413 | TrGAroCN | STYRENO2 + NO → $NO_2$ + $HO_2$ + HCHO + BENZAL | KRO2NO | Rickard and Pascoe (2009)* |
| G48414 | TrGAroCN | STYRENO2 + $NO_3$ → $NO_2$ + $HO_2$ + HCHO + BENZAL | KRO2NO3 | Rickard and Pascoe (2009)* |
| G48415 | TrGAroC | STYRENO2 → $HO_2$ + HCHO + BENZAL | k1_RO2sRO2 | Rickard and Pascoe (2009)* |
| G48416 | TrGAroC | STYRENOOH + OH → STYRENO2 | 6.16E-11 | Rickard and Pascoe (2009) |
| G49200 | TrGTerC | C96O2 → C97O2 | k1_RO2pRO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G49201 | TrGTerC | C96O2 + $HO_2$ → C96OOH | k_RO2_HO2(temp,9) | Rickard and Pascoe (2009) |
| G49202a | TrGTerCN | C96O2 + NO → C97O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(10,1,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G49202b | TrGTerCN | C96O2 + NO → C96NO3 | KRO2NO*alpha_AN(10,1,0,0,0, temp,cair) | Rickard and Pascoe (2009) |
| G49203 | TrGTerCN | C96NO3 + OH → NORPINAL + $NO_2$ | 2.88E-12 | Rickard and Pascoe (2009) |
| G49204a | TrGTerC | C96OOH + OH → C96O2 | k_ROOHRO | Rickard and Pascoe (2009) |
| G49205b | TrGTerC | C96OOH + OH → NORPINAL + OH | 1.30E-11 | Rickard and Pascoe (2009) |
| G49206 | TrGTerC | C97O2 → C98O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G49207 | TrGTerCN | C97O2 + NO → C98O2 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G49208a | TrGTerC | C97O2 + $HO_2$ → C97OOH | k_RO2_HO2(temp,9)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G49208b | TrGTerC | C97O2 + $HO_2$ → C98O2 + OH | k_RO2_HO2(temp,9)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G49209 | TrGTerC | C97OOH + OH → C97O2 | 1.05E-11 | Rickard and Pascoe (2009) |
| G49210 | TrGTerC | C98O2 → C614O2 + $CH_3COCH_3$ | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G49211a | TrGTerCN | C98O2 + NO → C614O2 + $CH_3COCH_3$ + $NO_2$ | KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G49211b | TrGTerCN | C98O2 + NO → 9 LCARBON + LNITROGEN | KRO2NO*alpha_AN(12,3,0,0,0, temp,cair) | Rickard and Pascoe (2009) |
| G49212 | TrGTerC | C98O2 + $HO_2$ → C98OOH | k_RO2_HO2(temp,9) | Rickard and Pascoe (2009) |
| G49213 | TrGTerC | C98OOH + OH → C98O2 | 2.05E-11 | Rickard and Pascoe (2009) |
| G49214 | TrGTerC | NORPINAL + OH → C85CO3 | 2.64E-11 | Rickard and Pascoe (2009) |
| G49215 | TrGTerCN | NORPINAL + $NO_3$ → C85CO3 + $HNO_3$ | KNO3AL*8.5 | Rickard and Pascoe (2009) |
| G49216 | TrGTerC | C85CO3 → C85O2 + $CO_2$ | k1_RO2RCO3 | Rickard and Pascoe (2009) |
| G49217 | TrGTerCN | C85CO3 + NO → C85O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G49218 | TrGTerCN | C85CO3 + $NO_2$ → C9PAN2 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G49219a | TrGTerC | C85CO3 + $HO_2$ → C85CO3H | KAPHO2*(r_CO3_OOH+r_CO3_O3) | Rickard and Pascoe (2009) |
| G49219b | TrGTerC | C85CO3 + $HO_2$ → C85O2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G49220 | TrGTerCN | C9PAN2 → C85CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G49221 | TrGTerCN | C9PAN2 + OH → C85OOH + CO + $NO_2$ | 6.60E-12 | Rickard and Pascoe (2009) |
| G49222 | TrGTerC | C85CO3H + OH → C85CO3 | 1.02E-11 | Rickard and Pascoe (2009) |
| G49223a | TrGTerC | C89CO3 → .8 C811CO3 + .2 C89O2 + .2 $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G49223b | TrGTerC | C89CO3 → C89CO2H | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G49224a | TrGTerC | C89CO3 + $HO_2$ → C89CO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G49224b | TrGTerC | C89CO3 + $HO_2$ → C89CO2H + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G49224c | TrGTerC | C89CO3 + $HO_2$ → .80 C811CO3 + .20 C89O2 + .2 $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G49225 | TrGTerCN | C89CO3 + $NO_2$ → C89PAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G49226 | TrGTerCN | C89CO3 + NO → .8 C811CO3 + .2 C89O2 + .2 $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G49227 | TrGTerC | C89CO2H + OH → .8 C811CO3 + .2 C89O2 + .2 $CO_2$ | 2.69E-11 | Rickard and Pascoe (2009) |
| G49228 | TrGTerC | C89CO3H + OH → C89CO3 | 3.00E-11 | Rickard and Pascoe (2009) |
| G49229 | TrGTerCN | C89PAN → C89CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G49230 | TrGTerCN | C89PAN + OH → $CH_3COCH_3$ + CO13C4CHO + CO + $NO_2$ | 2.52E-11 | Rickard and Pascoe (2009) |
| G49231a | TrGTerC | C811CO3 → C811O2 + $CO_2$ | k1_RO2RCO3*0.9 | Sander et al. (2019) |
| G49231b | TrGTerC | C811CO3 → PINIC | k1_RO2RCO3*0.1 | Sander et al. (2019) |
| G49232a | TrGTerC | C811CO3 + $HO_2$ → C811CO3H | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G49232b | TrGTerC | C811CO3 + $HO_2$ → PINIC + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G49232c | TrGTerC | C811CO3 + $HO_2$ → C811O2 + $CO_2$ + OH | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G49233 | TrGTerCN | C811CO3 + NO → C811O2 + $CO_2$ + $NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G49234 | TrGTerCN | C811CO3 + $NO_2$ → C811PAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G49235 | TrGTerC | PINIC + OH → C811O2 + $CO_2$ | 7.29E-12 | Rickard and Pascoe (2009) |
| G49236 | TrGTerC | NOPINONE + OH → NOPINDO2 | 1.55E-11 | Capouet et al. (2008), Rickard and Pascoe (2009) |
| G49237a | TrGTerC | NOPINDO2 + $HO_2$ → NOPINDOOH | k_RO2_HO2(temp,9)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G49237b | TrGTerC | NOPINDO2 + $HO_2$ → C89CO3 + OH | k_RO2_HO2(temp,9)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G49238 | TrGTerCN | NOPINDO2 + NO → C89CO3 + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G49239 | TrGTerC | NOPINDO2 → C89CO3 | k1_RO2pORO2 | Rickard and Pascoe (2009) |
| G49240 | TrGTerC | NOPINDOOH → NOPINDCO | 2.63E-11 | Rickard and Pascoe (2009) |
| G49241 | TrGTerC | NOPINDCO + OH → C89CO3 | 3.07E-12 | Rickard and Pascoe (2009) |
| G49242 | TrGTerC | NOPINOO → NOPINONE + $H_2O_2$ | 6.00E-18*c(ind_H2O) | Rickard and Pascoe (2009) |
| G49243 | TrGTerC | NOPINOO + CO → NOPINONE + $CO_2$ | 1.2E-15 | Rickard and Pascoe (2009) |
| G49244 | TrGTerCN | NOPINOO + NO → NOPINONE + $NO_2$ | 1.E-14 | Rickard and Pascoe (2009) |
| G49245 | TrGTerCN | NOPINOO + $NO_2$ → NOPINONE + $NO_3$ | 1.E-15 | Rickard and Pascoe (2009) |
| G49246 | TrGTerC | NORPINENOL + OH → HCOOH + OH + C86O2 | k_CH2CHOH_OH_HCOOH | Sander et al. (2019), So et al. (2014)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G49247 | TrGTerC | NORPINENOL + HCOOH → NORPINAL + HCOOH | k_CH2CHOH_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G49248 | TrGTerC | NORPINAL + HCOOH → NORPINENOL + HCOOH | k_ALD_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G49249 | TrGTerC | C811CO3H + OH → C811CO3 | 1.04E-11 | Rickard and Pascoe (2009) |
| G49250 | TrGTerCN | C811PAN → C811CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G49251 | TrGTerCN | C811PAN + OH → C721CHO + CO + $NO_2$ | 6.77E-12 | Rickard and Pascoe (2009) |
| G49400a | TrGAroC | LTMB + OH → TLEPOXMUC + $HO_2$ + 2 LCARBON | 0.827E-11 | Rickard and Pascoe (2009)* |
| G49400b | TrGAroC | LTMB + OH → C6H5CH2O2 + 2 LCARBON | 0.189E-11 | Rickard and Pascoe (2009)* |
| G49400c | TrGAroC | LTMB + OH → CRESOL + 2 LCARBON | 0.141E-11 | Rickard and Pascoe (2009)* |
| G49400d | TrGAroC | LTMB + OH → TLBIPERO2 + $HO_2$ + 2 LCARBON | 2.917E-11 | Rickard and Pascoe (2009)* |
| G49401 | TrGAroCN | LTMB + $NO_3$ → C6H5CH2O2 + $HNO_3$ + 2 LCARBON | 1.52E-15 | Rickard and Pascoe (2009)* |
| G40200 | TrGTerC | APINENE + OH → .75 LAPINABO2 + .15 MENTHEN6ONE + .15 $HO_2$ + .10 ROO6R1O2 | 1.2E-11*EXP(440./temp) | Atkinson et al. (2006)* |
| G40201a | TrGTerCN | LAPINABO2 + NO → PINAL + $HO_2$ + $NO_2$ | KRO2NO*(1.-(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair))) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40201b | TrGTerCN | LAPINABO2 + NO → LAPINABNO3 | KRO2NO*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40202a | TrGTerC | LAPINABO2 + $HO_2$ → LAPINABOOH | k_RO2_HO2(temp,10)*(1.-r_CHOHCH2O2_OH) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40202b | TrGTerC | LAPINABO2 + $HO_2$ → PINAL + $HO_2$ + OH | k_RO2_HO2(temp,10)*r_CHOHCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40203 | TrGTerC | LAPINABO2 → PINAL + $HO_2$ | RO2*(0.65*k1_RO2tORO2+.35*k1_RO2sORO2) | Rickard and Pascoe (2009)* |
| G40204 | TrGTerC | LAPINABOOH + OH → .35 LAPINABO2 + .65 C96CO3 | 2.77E-11 | Rickard and Pascoe (2009)* |
| G40205 | TrGTerCN | LAPINABNO3 + OH → .35 PINAL + .65 C96CO3 + $NO_2$ | 4.29E-12 | Rickard and Pascoe (2009)* |
| G40206 | TrGTerC | MENTHEN6ONE + OH → OHMENTHEN6ONEO2 | 6.46E-11 | Vereecken et al. (2007)* |
| G40207 | TrGTerCN | OHMENTHEN6ONEO2 + NO → 2OHMENTHEN6ONE + $HO_2$ + $NO_2$ | KRO2NO | Vereecken et al. (2007)* |
| G40208 | TrGTerC | OHMENTHEN6ONEO2 + $HO_2$ → 2OHMENTHEN6ONE | k_RO2_HO2(temp,10) | Vereecken et al. (2007) |
| G40209 | TrGTerC | OHMENTHEN6ONEO2 → 2OHMENTHEN6ONE + $HO_2$ | k1_RO2tORO2 | Vereecken et al. (2007) |
| G40210 | TrGTerC | 2OHMENTHEN6ONE + OH → 10 LCARBON | 1E-11 | Vereecken et al. (2007) |
| G40211 | TrGTerC | PINAL + OH → .772 C96CO3 + .228 PINALO2 | 5.2E-12*EXP(600./temp) | Wallington et al. (2018)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G40212 | TrGTerCN | PINAL + $NO_3$ → C96CO3 + $HNO_3$ | 2.0E-14 | Wallington et al. (2018)* |
| G40213a | TrGTerC | C96CO3 → C96O2 + $CO_2$ | k1_RO2RCO3*0.9 | Rickard and Pascoe (2009) |
| G40213b | TrGTerC | C96CO3 → PINONIC | k1_RO2RCO3*0.1 | Rickard and Pascoe (2009) |
| G40214a | TrGTerC | C96CO3 + $HO_2$ → PERPINONIC | KAPHO2*r_CO3_OOH | Rickard and Pascoe (2009) |
| G40214b | TrGTerC | C96CO3 + $HO_2$ → PINONIC + $O_3$ | KAPHO2*r_CO3_O3 | Rickard and Pascoe (2009) |
| G40214c | TrGTerC | C96CO3 + $HO_2$ → C96O2 + OH + $CO_2$ | KAPHO2*r_CO3_OH | Rickard and Pascoe (2009) |
| G40215 | TrGTerCN | C96CO3 + $NO_2$ → C10PAN2 | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G40216 | TrGTerCN | C96CO3 + NO → C96O2 + $NO_2$ + $CO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G40217 | TrGTerCN | C96CO3 + $NO_3$ → C96O2 + $NO_2$ + $CO_2$ | KRO2NO3*1.74 | Rickard and Pascoe (2009) |
| G40218 | TrGTerCN | C10PAN2 → C96CO3 + $NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G40219 | TrGTerCN | C10PAN2 + OH → NORPINAL + CO + $NO_2$ | 3.66E-12 | Rickard and Pascoe (2009) |
| G40220 | TrGTerC | PINONIC + OH → C96O2 + $CO_2$ | 6.65E-12 | Rickard and Pascoe (2009) |
| G40221 | TrGTerC | PERPINONIC + OH → C96CO3 | 9.73E-12 | Rickard and Pascoe (2009) |
| G40222 | TrGTerC | PINALO2 + $HO_2$ → PINALOOH | k_RO2_HO2(temp,10) | Rickard and Pascoe (2009) |
| G40223a | TrGTerCN | PINALO2 + NO → C106O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(12,3,0,1,0, temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40223b | TrGTerCN | PINALO2 + NO → PINALNO3 | KRO2NO*alpha_AN(12,3,0,1,0, temp,cair) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40224 | TrGTerC | PINALO2 → C106O2 | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G40225 | TrGTerC | PINALOOH + OH → PINALO2 | 2.75E-11 | Rickard and Pascoe (2009) |
| G40226 | TrGTerCN | PINALNO3 + OH → CO235C6CHO + $CH_3COCH_3$ + $NO_2$ | 2.25E-11 | Rickard and Pascoe (2009) |
| G40227 | TrGTerC | C106O2 + $HO_2$ → C106OOH | k_RO2_HO2(temp,10) | Rickard and Pascoe (2009) |
| G40228a | TrGTerCN | C106O2 + NO → C716O2 + $CH_3COCH_3$ + $NO_2$ | KRO2NO*0.875*(1.-alpha_AN(13,3,0, 0,0,temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40228b | TrGTerCN | C106O2 + NO → C106NO3 | KRO2NO*0.875*alpha_AN(13,3,0,0, 0,temp,cair) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40229 | TrGTerC | C106O2 → C716O2 + $CH_3COCH_3$ | k1_RO2tRO2 | Rickard and Pascoe (2009) |
| G40230 | TrGTerC | C106OOH + OH → C106O2 | 8.01E-11 | Rickard and Pascoe (2009) |
| G40231 | TrGTerCN | C106NO3 + OH → CO235C6CHO + $CH_3COCH_3$ + $NO_2$ | 7.03E-11 | Rickard and Pascoe (2009) |
| G40232 | TrGTerC | APINENE + $O_3$ → .09 APINBOO + .08 PINONIC + .77 OH + .33 NORPINAL + .33 CO + .33 $HO_2$ + .06 APINAOO + .44 C109O2 | 8.05E-16*EXP(-640./temp) | Wallington et al. (2018)* |
| G40233 | TrGTerC | APINAOO → PINAL + $H_2O_2$ | 1.00E-17*c(ind_H2O) | Rickard and Pascoe (2009) |
| G40234 | TrGTerC | APINAOO + CO → PINAL + $CO_2$ | 1.20E-15 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G40235 | TrGTerCN | APINAOO + NO → PINAL + $NO_2$ | 1.00E-14 | Rickard and Pascoe (2009) |
| G40236 | TrGTerCN | APINAOO + $NO_2$ → PINAL + $NO_3$ | 1.00E-15 | Rickard and Pascoe (2009) |
| G40237a | TrGTerC | APINBOO → PINONIC | 1.00E-17*c(ind_H2O)*(0.08+0.15) | Rickard and Pascoe (2009) |
| G40237b | TrGTerC | APINBOO → PINAL + $H_2O_2$ | 1.00E-17*c(ind_H2O)*0.77 | Rickard and Pascoe (2009) |
| G40238 | TrGTerC | APINBOO + CO → PINAL + $CO_2$ | 1.20E-15 | Rickard and Pascoe (2009) |
| G40239 | TrGTerCN | APINBOO + NO → PINAL + $NO_2$ | 1.00E-14 | Rickard and Pascoe (2009) |
| G40240 | TrGTerCN | APINBOO + $NO_2$ → PINAL + $NO_3$ | 1.00E-15 | Rickard and Pascoe (2009) |
| G40241 | TrGTerC | C109O2 → C89CO3 + HCHO | k1_RO2pORO2 | Rickard and Pascoe (2009) |
| G40242 | TrGTerCN | C109O2 + NO → C89CO3 + HCHO + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G40243a | TrGTerC | C109O2 + $HO_2$ → C109OOH | k_RO2_HO2(temp,10)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40243b | TrGTerC | C109O2 + $HO_2$ → C89CO3 + HCHO + OH | k_RO2_HO2(temp,10)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40244 | TrGTerC | C109OOH + OH → C109CO + OH | 5.47E-11 | Rickard and Pascoe (2009) |
| G40245 | TrGTerC | C109CO + OH → C89CO3 + CO | 5.47E-11 | Rickard and Pascoe (2009) |
| G40246 | TrGTerCN | APINENE + $NO_3$ → LNAPINABO2 | 1.2E-12*EXP(490./temp) | Wallington et al. (2018)* |
| G40247 | TrGTerCN | LNAPINABO2 → PINAL + $NO_2$ | (0.65*k1_RO2tRO2 + 0.35*k1_ RO2sRO2) | Rickard and Pascoe (2009) |
| G40248 | TrGTerCN | LNAPINABO2 + NO → PINAL + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G40249 | TrGTerCN | LNAPINABO2 + $HO_2$ → LNAPINABOOH | k_RO2_HO2(temp,10) | Rickard and Pascoe (2009) |
| G40250 | TrGTerCN | LNAPINABO2 + $NO_3$ → PINAL + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G40251 | TrGTerCN | LNAPINABOOH + OH → LNAPINABO2 | (.65*6.87E-12+.35*1.23E-11) | Rickard and Pascoe (2009) |
| G40252a | TrGTerC | BPINENE + OH → BPINAO2 | 1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068) | Gill and Hites (2002)* |
| G40252b | TrGTerC | BPINENE + OH → ROO6R1O2 | 1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068) | Gill and Hites (2002)* |
| G40253a | TrGTerC | BPINAO2 + $HO_2$ → BPINAOOH | k_RO2_HO2(temp,10)*r_COCH2O2_OOH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40253b | TrGTerC | BPINAO2 + $HO_2$ → NOPINONE + HCHO + $HO_2$ + OH | k_RO2_HO2(temp,10)*r_COCH2O2_OH | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40254a | TrGTerCN | BPINAO2 + NO → NOPINONE + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(11,3,0,0,0, temp,cair)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40254b | TrGTerCN | BPINAO2 + NO → BPINANO3 | KRO2NO*alpha_AN(11,3,0,0,0, temp,cair) | Rickard and Pascoe (2009), Sander et al. (2019) |
| G40255 | TrGTerC | BPINAO2 → NOPINONE + HCHO + $HO_2$ | k1_RO2tORO2 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G40256 | TrGTerC | BPINAOOH + OH → BPINAO2 | 1.33E-11 | Rickard and Pascoe (2009) |
| G40257 | TrGTerCN | BPINANO3 + OH → NOPINONE + HCHO + $NO_2$ | 4.70E-12 | Rickard and Pascoe (2009) |
| G40258a | TrGTerCN | ROO6R1O2 + NO → ROO6R3O2 + $CH_3COCH_3$ + $NO_2$ | KRO2NO*(1.-alpha_AN(13,3,0,0,0, temp,cair)) | Vereecken and Peeters (2012) |
| G40258b | TrGTerCN | ROO6R1O2 + NO → ROO6R1NO3 | KRO2NO*alpha_AN(13,3,0,0,0, temp,cair) | Vereecken and Peeters (2012) |
| G40259 | TrGTerC | ROO6R1O2 + $HO_2$ → 10 LCARBON | k_RO2_HO2(temp,10) | Vereecken and Peeters (2012)* |
| G40260 | TrGTerC | ROO6R1O2 → ROO6R3O2 + $CH_3COCH_3$ | k1_RO2tORO2 | Vereecken and Peeters (2012) |
| G40261a | TrGTerCN | RO6R1O2 + NO → RO6R3O2 + $NO_2$ | KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair)) | Vereecken and Peeters (2012) |
| G40261b | TrGTerCN | RO6R1O2 + NO → RO6R1NO3 | KRO2NO*alpha_AN(12,3,0,0,0, temp,cair) | Vereecken and Peeters (2012) |
| G40262 | TrGTerC | RO6R1O2 + $HO_2$ → 10 LCARBON | k_RO2_HO2(temp,10) | Vereecken and Peeters (2012)* |
| G40263 | TrGTerC | RO6R1O2 → RO6R3O2 | k1_RO2sORO2 | Vereecken and Peeters (2012) |
| G40264a | TrGTerCN | RO6R3O2 + NO → 9 LCARBON + HCHO + $HO_2$ + $NO_2$ | KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair)) | Vereecken and Peeters (2012) |
| G40264b | TrGTerCN | RO6R3O2 + NO → 10 LCARBON + LNITROGEN | KRO2NO*alpha_AN(12,3,0,0,0, temp,cair) | Vereecken and Peeters (2012) |
| G40265 | TrGTerC | RO6R3O2 + $HO_2$ → 10 LCARBON | k_RO2_HO2(temp,10) | Vereecken and Peeters (2012) |
| G40266 | TrGTerC | RO6R3O2 → 9 LCARBON + HCHO + $HO_2$ | k1_RO2sRO2 | Vereecken and Peeters (2012)* |
| G40267a | TrGTerC | BPINENE + $O_3$ → NOPINONE + .63 CO + .37 $CH_2OO$ + .16 OH + .16 $HO_2$ | 1.35E-15*EXP(-1270./temp) *.051/(1.-.027) | Wallington et al. (2018)* |
| G40267b | TrGTerC | BPINENE + $O_3$ → NOPINOO + $CO_2$ | 1.35E-15*EXP(-1270./temp) *.368/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40267c | TrGTerC | BPINENE + $O_3$ → NOPINDO2 + $CO_2$ + OH | 1.35E-15*EXP(-1270./temp) *.283/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40267d | TrGTerC | BPINENE + $O_3$ → C8BC + 2 $CO_2$ | 1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40268 | TrGTerCN | BPINENE + $NO_3$ → LNBPINABO2 | 2.51E-12 | Wallington et al. (2018)* |
| G40269 | TrGTerCN | LNBPINABO2 + $HO_2$ → LNBPINABOOH | k_RO2_HO2(temp,10) | Rickard and Pascoe (2009) |
| G40270 | TrGTerCN | LNBPINABO2 + NO → NOPINONE + HCHO + $NO_2$ + $NO_2$ | KRO2NO | Rickard and Pascoe (2009)* |
| G40271 | TrGTerCN | LNBPINABO2 + $NO_3$ → NOPINONE + HCHO + $NO_2$ + $NO_2$ | KRO2NO3 | Rickard and Pascoe (2009) |
| G40272a | TrGTerCN | LNBPINABO2 → NOPINONE + HCHO + $NO_2$ | k1_RO2tRO2*0.7 | Rickard and Pascoe (2009) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G40272b | TrGTerCN | LNBPINABO2 → BPINANO3 | k1_RO2tRO2*0.3 | Rickard and Pascoe (2009) |
| G40273 | TrGTerCN | LNBPINABOOH + OH → LNBPINABO2 | 9.58E-12 | Rickard and Pascoe (2009) |
| G40274 | TrGTerCN | ROO6R1NO3 + OH → ROO6R3O2 + $CH_3COCH_3$ + $NO_2$ | 9.16E-13 | Vereecken and Peeters (2012), Gill and Hites (2002)* |
| G40275 | TrGTerCN | RO6R1NO3 + OH → 9 LCARBON + HCHO + $HO_2$ + $NO_2$ | 9.16E-13 | Vereecken and Peeters (2012), Gill and Hites (2002) |
| G40276 | TrGTerC | PINEOL + OH → HCOOH + OH + NORPINAL | k_CH2CHOH_OH_HCOOH | Sander et al. (2019), So et al. (2014)* |
| G40277 | TrGTerC | PINEOL + HCOOH → PINAL + HCOOH | k_CH2CHOH_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G40278 | TrGTerC | PINAL + HCOOH → PINEOL + HCOOH | k_ALD_HCOOH | Sander et al. (2019), da Silva (2010)* |
| G40279a | TrGC | CARENE + OH → LAPINABO2 | 8.8E-11*(.50+.25) | Atkinson and Arey (2003) |
| G40279b | TrGC | CARENE + OH → MENTHEN6ONE + $HO_2$ | 8.8E-11*.25*.60 | Atkinson and Arey (2003) |
| G40279c | TrGC | CARENE + OH → ROO6R1O2 | 8.8E-11*.25*.40 | Atkinson and Arey (2003) |
| G40280a | TrGC | CARENE + $O_3$ → APINBOO | 3.7E-17*.50*.18 | Atkinson and Arey (2003) |
| G40280b | TrGC | CARENE + $O_3$ → PINONIC | 3.7E-17*.50*.16 | Atkinson and Arey (2003) |
| G40280c | TrGC | CARENE + $O_3$ → OH + NORPINAL + CO + $HO_2$ | 3.7E-17*.50*.66 | Atkinson and Arey (2003) |
| G40280d | TrGC | CARENE + $O_3$ → APINAOO | 3.7E-17*.50*.12 | Atkinson and Arey (2003) |
| G40280e | TrGC | CARENE + $O_3$ → OH + C109O2 | 3.7E-17*.50*(.22+.66) | Atkinson and Arey (2003) |
| G40281 | TrGCN | CARENE + $NO_3$ → LNAPINABO2 | 9.1E-12 | Atkinson and Arey (2003) |
| G40282a | TrGTerC | SABINENE + OH → BPINAO2 | 1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068) | Gill and Hites (2002)* |
| G40282b | TrGTerC | SABINENE + OH → ROO6R1O2 | 1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068) | Vereecken and Peeters (2012), Gill and Hites (2002)* |
| G40283a | TrGTerC | SABINENE + $O_3$ → NOPINONE + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 $HO_2$ | 1.35E-15*EXP(-1270./temp) *.051/(1.-.027) | Wallington et al. (2018)* |
| G40283b | TrGTerC | SABINENE + $O_3$ → NOPINOO + $CO_2$ | 1.35E-15*EXP(-1270./temp) *.368/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40283c | TrGTerC | SABINENE + $O_3$ → NOPINDO2 + $CO_2$ + OH | 1.35E-15*EXP(-1270./temp) *.283/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40283d | TrGTerC | SABINENE + $O_3$ → C8BC + 2 $CO_2$ | 1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40284 | TrGTerCN | SABINENE + $NO_3$ → LNBPINABO2 | 2.51E-12 | Wallington et al. (2018)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G40285a | TrGTerC | CAMPHENE + OH → BPINAO2 | 1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068) | Gill and Hites (2002)* |
| G40285b | TrGTerC | CAMPHENE + OH → ROO6R1O2 | 1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068) | Vereecken and Peeters (2012), Gill and Hites (2002)* |
| G40286a | TrGTerC | CAMPHENE + $O_3$ → NOPINONE + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 $HO_2$ | 1.35E-15*EXP(-1270./temp) *.051/(1.-.027) | Wallington et al. (2018)* |
| G40286b | TrGTerC | CAMPHENE + $O_3$ → NOPINOO + $CO_2$ | 1.35E-15*EXP(-1270./temp) *.368/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40286c | TrGTerC | CAMPHENE + $O_3$ → NOPINDO2 + $CO_2$ + OH | 1.35E-15*EXP(-1270./temp) *.283/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40286d | TrGTerC | CAMPHENE + $O_3$ → C8BC + 2 $CO_2$ | 1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027) | Nguyen et al. (2009), Wallington et al. (2018) |
| G40287 | TrGTerCN | CAMPHENE + $NO_3$ → LNBPINABO2 | 2.51E-12 | Wallington et al. (2018)* |
| G40400 | TrGAroC | LHAROM + OH → .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + .18 $HO_2$ + 4 LCARBON | 5.67E-11 | Rickard and Pascoe (2009)* |
| G40401 | TrGAroCN | LHAROM + $NO_3$ → C6H5CH2O2 + $HNO_3$ + 4 LCARBON | 2.60E-15 | Rickard and Pascoe (2009)* |
| G6100 | UpStTrGCl | Cl + $O_3$ → ClO + $O_2$ | 2.8E-11*EXP(-250./temp) | Atkinson et al. (2007) |
| G6101 | UpStGCl | ClO + $O(^3P)$ → Cl + $O_2$ | 2.5E-11*EXP(110./temp) | Atkinson et al. (2007) |
| G6102a | StTrGCl | ClO + ClO → $Cl_2$ + $O_2$ | 1.0E-12*EXP(-1590./temp) | Atkinson et al. (2007) |
| G6102b | StTrGCl | ClO + ClO → 2 Cl + $O_2$ | 3.0E-11*EXP(-2450./temp) | Atkinson et al. (2007) |
| G6102c | StTrGCl | ClO + ClO → Cl + OClO | 3.5E-13*EXP(-1370./temp) | Atkinson et al. (2007) |
| G6102d | StTrGCl | ClO + ClO → $Cl_2O_2$ | k_ClO_ClO | Burkholder et al. (2015) |
| G6103 | StTrGCl | $Cl_2O_2$ → ClO + ClO | k_ClO_ClO/(2.16E-27*EXP(8537./ temp)) | Burkholder et al. (2015)* |
| G6200 | StGCl | Cl + $H_2$ → HCl + H | 3.9E-11*EXP(-2310./temp) | Atkinson et al. (2007) |
| G6201a | StGCl | Cl + $HO_2$ → HCl + $O_2$ | 4.4E-11-7.5E-11*EXP(-620./temp) | Atkinson et al. (2007) |
| G6201b | StGCl | Cl + $HO_2$ → ClO + OH | 7.5E-11*EXP(-620./temp) | Atkinson et al. (2007) |
| G6202 | StTrGCl | Cl + $H_2O_2$ → HCl + $HO_2$ | 1.1E-11*EXP(-980./temp) | Atkinson et al. (2007) |
| G6203 | StGCl | ClO + OH → .94 Cl + .94 $HO_2$ + .06 HCl + .06 $O_2$ | 7.3E-12*EXP(300./temp) | Atkinson et al. (2007) |
| G6204 | StTrGCl | ClO + $HO_2$ → HOCl + $O_2$ | 2.2E-12*EXP(340./temp) | Atkinson et al. (2007)* |
| G6205 | StTrGCl | HCl + OH → Cl + $H_2O$ | 1.7E-12*EXP(-230./temp) | Atkinson et al. (2007) |
| G6206 | StGCl | HOCl + OH → ClO + $H_2O$ | 3.0E-12*EXP(-500./temp) | Burkholder et al. (2015) |
| G6300 | UpStTrGClN | ClO + NO → $NO_2$ + Cl | 6.2E-12*EXP(295./temp) | Atkinson et al. (2007) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G6301 | StTrGClN | $ClO + NO_2 \rightarrow ClNO_3$ | k_3rd_iupac(temp,cair,1.6E-31, 3.4,7.E-11,0.,0.4) | Atkinson et al. (2007) |
| G6302 | TrGClN | $ClNO_3 \rightarrow ClO + NO_2$ | 6.918E-7*EXP(-10909./temp)*cair | Anderson and Fahey (1990) |
| G6303 | StGClN | $ClNO_3 + O(^3P) \rightarrow ClO + NO_3$ | 4.5E-12*EXP(-900./temp) | Atkinson et al. (2007) |
| G6304 | StTrGClN | $ClNO_3 + Cl \rightarrow Cl_2 + NO_3$ | 6.2E-12*EXP(145./temp) | Atkinson et al. (2007) |
| G6400 | StTrGCl | $Cl + CH_4 \rightarrow HCl + CH_3$ | 6.6E-12*EXP(-1240./temp) | Atkinson et al. (2006) |
| G6401 | StTrGCl | $Cl + HCHO \rightarrow HCl + CO + HO_2$ | 8.1E-11*EXP(-34./temp) | Atkinson et al. (2006) |
| G6402 | StTrGCl | $Cl + CH_3OOH \rightarrow HCHO + HCl + OH$ | 5.9E-11 | Atkinson et al. (2006)* |
| G6403 | StTrGCl | $ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$ | 1.8E-12*EXP(-600./temp) | Burkholder et al. (2015) |
| G6404 | StGCl | $CCl_4 + O(^1D) \rightarrow$ LCARBON + ClO + 3 Cl | 3.3E-10 | Burkholder et al. (2015) |
| G6405 | StGCl | $CH_3Cl + O(^1D) \rightarrow 0.1\ CH_3Cl + 0.1\ O(^3P) + 0.46\ ClO + 0.35\ Cl + 0.09\ H + 0.9$ LCARBON + 0.09 LCHLORINE | 1.65E-10 | Burkholder et al. (2015) |
| G6406 | StGCl | $CH_3Cl + OH \rightarrow$ LCARBON + $H_2O$ + Cl | 1.96E-12*EXP(-1200./temp) | Burkholder et al. (2015) |
| G6407 | StGCCl | $CH_3CCl_3 + O(^1D) \rightarrow 2$ LCARBON + OH + 3 Cl | 3.25E-10 | Burkholder et al. (2015) |
| G6408 | StTrGCCl | $CH_3CCl_3 + OH \rightarrow 2$ LCARBON + $H_2O$ + 3 Cl | 1.64E-12*EXP(-1520./temp) | Burkholder et al. (2015) |
| G6409 | TrGCCl | $Cl + C_2H_4 \rightarrow HOCH_2CH_2O_2 + HCl$ | k_3rd_iupac(temp,cair,1.85E-29, 3.3,6.0E-10,0.0,0.4) | Atkinson et al. (2006)* |
| G6410 | TrGCCl | $Cl + CH_3CHO \rightarrow HCl + CH_3C(O)$ | 8.0e-11 | Atkinson et al. (2006) |
| G6411 | TrGCCl | $C_2H_2 + Cl \rightarrow$ LCARBON + $CH_3$ + HCl | k_3rd_iupac(temp,cair,6.1e-30, 3.0,2.0e-10,0.,0.6) | Atkinson et al. (2006) |
| G6412 | TrGCCl | $C_2H_6 + Cl \rightarrow C_2H_5O_2 + HCl$ | 8.3E-11*EXP(-100./temp) | Atkinson et al. (2006) |
| G6413 | StTrGClN | $Cl + CH_3ONO_2 \rightarrow HCl + HCHO + NO_2$ | 1.3E-11*EXP(-1200./temp) | Burkholder et al. (2015) |
| G6414 | StTrGClN | $Cl + CH_3ONO \rightarrow HCl + HCHO + NO$ | 2.1E-12 | Sokolov et al. (1999) |
| G6415 | StTrGCl | $Cl + CH_3O_2 \rightarrow .5\ ClO + .5\ CH_3O + .5\ HCl + .5\ CH_2OO$ | 1.6E-10 | Burkholder et al. (2015) |
| G6416 | TrGCClN | $Cl + CH_3CN \rightarrow NCCH_2O_2 + HCl$ | 1.6E-11*EXP(-2104./temp) | Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019) |
| G6500 | StGClF | $CF_2Cl_2 + O(^1D) \rightarrow$ LCARBON + 2 LFLUORINE + ClO + Cl | 1.4E-10 | Burkholder et al. (2015) |
| G6501 | StGClF | $CFCl_3 + O(^1D) \rightarrow$ LCARBON + LFLUORINE + ClO + 2 Cl | 2.3E-10 | Burkholder et al. (2015) |
| G7100 | StTrGBr | $Br + O_3 \rightarrow BrO + O_2$ | 1.7E-11*EXP(-800./temp) | Atkinson et al. (2007) |
| G7101 | StGBr | $BrO + O(^3P) \rightarrow Br + O_2$ | 1.9E-11*EXP(230./temp) | Atkinson et al. (2007) |
| G7102a | StTrGBr | $BrO + BrO \rightarrow 2\ Br + O_2$ | 2.7E-12 | Atkinson et al. (2007) |
| G7102b | StTrGBr | $BrO + BrO \rightarrow Br_2 + O_2$ | 2.9E-14*EXP(840./temp) | Atkinson et al. (2007) |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G7200 | StTrGBr | Br + $HO_2$ → HBr + $O_2$ | 7.7E-12*EXP(-450./temp) | Atkinson et al. (2007) |
| G7201 | StTrGBr | BrO + $HO_2$ → HOBr + $O_2$ | 4.5E-12*EXP(500./temp) | Atkinson et al. (2007) |
| G7202 | StTrGBr | HBr + OH → Br + $H_2O$ | 6.7E-12*EXP(155./temp) | Atkinson et al. (2007) |
| G7203 | StGBr | HOBr + $O(^3P)$ → OH + BrO | 1.2E-10*EXP(-430./temp) | Atkinson et al. (2007) |
| G7204 | StTrGBr | $Br_2$ + OH → HOBr + Br | 2.0E-11*EXP(240./temp) | Atkinson et al. (2007) |
| G7300 | TrGBrN | Br + $BrNO_3$ → $Br_2$ + $NO_3$ | 4.9E-11 | Orlando and Tyndall (1996) |
| G7301 | StTrGBrN | BrO + NO → Br + $NO_2$ | 8.7E-12*EXP(260./temp) | Atkinson et al. (2007) |
| G7302 | StTrGBrN | BrO + $NO_2$ → $BrNO_3$ | k_BrO_NO2 | Atkinson et al. (2007)* |
| G7303 | TrGBrN | $BrNO_3$ → BrO + $NO_2$ | k_BrO_NO2/(5.44E-9*EXP(14192./temp)*1.E6*R_gas*temp/(atm2Pa*N_A)) | Orlando and Tyndall (1996), Atkinson et al. (2007)* |
| G7400 | StTrGBr | Br + HCHO → HBr + CO + $HO_2$ | 7.7E-12*EXP(-580./temp) | Atkinson et al. (2006) |
| G7401 | TrGBr | Br + $CH_3OOH$ → $CH_3O_2$ + HBr | 2.6E-12*EXP(-1600./temp) | Kondo and Benson (1984) |
| G7402 | TrGBr | BrO + $CH_3O_2$ → HOBr + $CH_2OO$ | 2.42E-14*EXP(1617./temp) | Shallcross et al. (2015) |
| G7403 | StTrGBr | $CH_3Br$ + OH → LCARBON + $H_2O$ + Br | 1.42E-12*EXP(-1150./temp) | Burkholder et al. (2015) |
| G7404 | TrGBrC | Br + $C_2H_4$ → $HOCH_2CH_2O_2$ + HBr | 2.8E-13*EXP(224./temp)/(1.+1.13E24*EXP(-3200./temp)/C(ind_O2)) | Atkinson et al. (2006)* |
| G7405 | TrGBrC | Br + $CH_3CHO$ → HBr + $CH_3C(O)$ | 1.8e-11*EXP(-460./temp) | Atkinson et al. (2006) |
| G7406 | TrGBrC | Br + $C_2H_2$ → LCARBON + $CH_3O_2$ + HBr | 6.35e-15*EXP(440./temp) | Atkinson et al. (2006) |
| G7407 | TrGBr | $CHBr_3$ + OH → LCARBON + $H_2O$ + 3 Br | 9.0E-13*EXP(-360./temp) | Burkholder et al. (2015)* |
| G7408 | TrGBr | $CH_2Br_2$ + OH → LCARBON + $H_2O$ + 2 Br | 2.0E-12*EXP(-840./temp) | Burkholder et al. (2015)* |
| G7600 | TrGBrCl | Br + BrCl → $Br_2$ + Cl | 3.32E-15 | Manion et al. (2015) |
| G7601 | TrGBrCl | Br + $Cl_2$ → BrCl + Cl | 1.10E-15 | Dolson and Leone (1987) |
| G7602 | TrGBrCl | $Br_2$ + Cl → BrCl + Br | 2.3E-10*EXP(135./temp) | Bedjanian et al. (1998) |
| G7603a | StTrGBrCl | BrO + ClO → Br + OClO | 1.6E-12*EXP(430./temp) | Atkinson et al. (2007) |
| G7603b | StTrGBrCl | BrO + ClO → Br + Cl + $O_2$ | 2.9E-12*EXP(220./temp) | Atkinson et al. (2007) |
| G7603c | StTrGBrCl | BrO + ClO → BrCl + $O_2$ | 5.8E-13*EXP(170./temp) | Atkinson et al. (2007) |
| G7604 | TrGBrCl | BrCl + Cl → Br + $Cl_2$ | 1.45E-11 | Clyne and Cruse (1972) |
| G7605 | TrGBrCl | $CHCl_2Br$ + OH → LCARBON + 2 Cl + $H_2O$ + Br | 2.0E-12*EXP(-840./temp) | see note* |
| G7606 | TrGBrCl | $CHClBr_2$ + OH → LCARBON + Cl + $H_2O$ + 2 Br | 2.0E-12*EXP(-840./temp) | see note* |
| G7607 | TrGBrCl | $CH_2ClBr$ + OH → LCARBON + Cl + $H_2O$ + Br | 2.1E-12*EXP(-880./temp) | Burkholder et al. (2015)* |
| G8100 | TrGI | I + $O_3$ → IO + $O_2$ | 2.1E-11*EXP(-830./temp) | Atkinson et al. (2007) |
| G8102 | TrGI | OIO + OIO → I(part) | 5.E-11 | von Glasow et al. (2002)* |
| G8103 | TrGI | IO + IO → .38 OIO + 1.62 I + .62 $O_2$ | 5.4E-11*EXP(180./temp) | Atkinson et al. (2007)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G8200 | TrGI | $I + HO_2 \rightarrow HI + O_2$ | 1.5E-11*EXP(-1090./temp) | Atkinson et al. (2007) |
| G8201 | TrGI | $IO + HO_2 \rightarrow HOI + O_2$ | 1.4E-11*EXP(540./temp) | Atkinson et al. (2007) |
| G8202 | TrGI | $HI + OH \rightarrow I + H_2O$ | 1.6E-11*EXP(440./temp) | Atkinson et al. (2007) |
| G8203 | TrGI | $OIO + OH \rightarrow HIO_3$ | 2.2E-10*EXP(243./temp) | Plane et al. (2006) |
| G8204 | TrGI | $I_2 + OH \rightarrow HOI + I$ | 2.1E-10 | Atkinson et al. (2007) |
| G8205 | TrGI | $HOI + OH \rightarrow IO + H_2O$ | 5.0E-12 | Riffault et al. (2005) |
| G8300 | TrGIN | $I + NO_2 \rightarrow INO_2$ | k_I_NO2 | Atkinson et al. (2007)* |
| G8301 | TrGIN | $I + NO_3 \rightarrow IO + NO_2$ | 1.E-10 | Dillon et al. (2008) |
| G8302 | TrGIN | $IO + NO \rightarrow I + NO_2$ | 7.15E-12*EXP(300./temp) | Atkinson et al. (2007) |
| G8303 | TrGIN | $IO + NO_2 \rightarrow INO_3$ | k_3rd_iupac(temp,cair,7.7E-31, 5.,1.6E-11,0.,0.4) | Atkinson et al. (2007) |
| G8304 | TrGIN | $OIO + NO \rightarrow NO_2 + IO$ | 1.1E-12*EXP(542./temp) | Atkinson et al. (2007) |
| G8305 | TrGIN | $INO_2 \rightarrow I + NO_2$ | k_I_NO2/(3.7E-7*EXP(9568./temp) *1.E6*R_gas*temp/(atm2Pa*N_A)) | van den Bergh and Troe (1976), Atkinson et al. (2007)* |
| G8306 | TrGIN | $INO_3 \rightarrow IO + NO_2$ | 2.1e15*EXP(-13670./temp) | Kaltsoyannis and Plane (2008) |
| G8307 | TrGIN | $I_2 + NO_3 \rightarrow I + INO_3$ | 1.5E-12 | Atkinson et al. (2007) |
| G8308 | TrGIN | $IO + NO_3 \rightarrow OIO + NO_2$ | 9.E-12 | Dillon et al. (2008) |
| G8309 | TrGIN | $I + INO_3 \rightarrow I_2 + NO_3$ | 9.1E-11*EXP(-146./temp) | Kaltsoyannis and Plane (2008) |
| G8400 | TrGCI | $CH_3CHICH_3 + OH \rightarrow 2\ LCARBON + CH_3O_2 + I$ | 1.22E-12 | Carl and Crowley (2001) |
| G8401 | TrGI | $CH_3O_2 + IO \rightarrow .4\ I + .6\ OIO + HCHO + HO_2$ | 2.E-12 | Dillon et al. (2006b), Bale et al. (2005)* |
| G8402 | TrGIN | $CH_3I + NO_3 \rightarrow HNO_3 + HCHO + IO$ | 3.4E-17 | Wayne et al. (1991)* |
| G8600 | TrGClI | $IO + ClO \rightarrow .2\ ICl + .25\ Cl + .55\ OClO + .8\ I + .45\ O_2$ | 4.7E-12*EXP(280./temp) | Atkinson et al. (2007) |
| G8700 | TrGBrI | $I + BrO \rightarrow IO + Br$ | 1.2E-11 | Burkholder et al. (2015) |
| G8701 | TrGBrI | $IO + BrO \rightarrow Br + .8\ OIO + .2\ I + .2\ O_2$ | 1.5E-11*EXP(510./temp) | Atkinson et al. (2007)* |
| G8702 | TrGBrI | $IBr + OH \rightarrow .84\ HOI + .84\ Br + .16\ HOBr + .16\ I$ | 1.4E-10 | Riffault et al. (2005) |
| G8703 | TrGBrI | $IO + Br \rightarrow I + BrO$ | 2.3E-11 | Bedjanian et al. (1997) |
| G8704 | TrGBrI | $I_2 + Br \rightarrow IBr + I$ | 1.2E-10 | Bedjanian et al. (1997) |
| G9200 | StTrGS | $SO_2 + OH \rightarrow H_2SO_4 + HO_2$ | k_3rd(temp,cair,3.3E-31,4.3, 1.6E-12,0.,0.6) | Burkholder et al. (2015) |
| G9400a | TrGCS | $DMS + OH \rightarrow CH_3SO_2 + HCHO$ | 1.13E-11*EXP(-253./temp) | Atkinson et al. (2004)* |
| G9400b | TrGCS | $DMS + OH \rightarrow DMSO + HO_2$ | k_DMS_OH | Atkinson et al. (2004)* |
| G9401 | TrGCNS | $DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$ | 1.9E-13*EXP(520./temp) | Atkinson et al. (2004) |
| G9402 | TrGCS | $DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3 + .4\ HO_2 + .4\ CH_3SO_3H$ | 1.E-10 | Hynes and Wine (1996)* |

Table 1: Gas phase reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| G9403 | TrGS | $CH_3SO_2 \rightarrow SO_2 + CH_3$ | 1.8E13*EXP(-8661./temp) | Barone et al. (1995) |
| G9404 | TrGS | $CH_3SO_2 + O_3 \rightarrow CH_3SO_3$ | 3.E-13 | Barone et al. (1995) |
| G9405 | TrGS | $CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$ | 5.E-11 | Barone et al. (1995) |
| G9408 | StTrGS | $CH_2OO + SO_2 \rightarrow H_2SO_4 + HCHO$ | k_CH2OO_SO2 | Welz et al. (2012), Stone et al. (2014)* |
| G9409 | TrGTerCS | $NOPINOO + SO_2 \rightarrow NOPINONE + H_2SO_4$ | 7.E-14 | Rickard and Pascoe (2009) |
| G9410 | TrGTerCS | $APINAOO + SO_2 \rightarrow PINAL + H_2SO_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G9411 | TrGTerCS | $APINBOO + SO_2 \rightarrow PINAL + H_2SO_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G9412 | TrGTerCS | $MBOOO + SO_2 \rightarrow IBUTALOH + H_2SO_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G9600 | TrGCClS | $DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$ | 3.3E-10 | Atkinson et al. (2004) |
| G9700 | TrGBrCS | $DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$ | 9.E-11*EXP(-2386./temp) | Jefferson et al. (1994) |
| G9701 | TrGBrCS | $DMS + BrO \rightarrow DMSO + Br$ | 4.4E-13 | Ingham et al. (1999) |
| G9800 | TrGCIS | $DMS + IO \rightarrow DMSO + I$ | 3.2E-13*EXP(-925./temp) | Dillon et al. (2006a) |
| G10100 | TrGHg | $Hg + O_3 \rightarrow HgO + O_2$ | 3.0E-20 | Hall (1995) |
| G10200 | TrGHg | $Hg + OH \rightarrow HgO + H$ | 3.55E-14*EXP(294./temp) | Pal and Ariya (2004) |
| G10201 | TrGHg | $Hg + H_2O_2 \rightarrow HgO + H_2O$ | 8.5E-19 | Tokos et al. (1998)* |
| G10600 | TrGClHg | $Hg + Cl \rightarrow HgCl$ | 1.0E-11 | Ariya et al. (2002) |
| G10601 | TrGClHg | $Hg + Cl_2 \rightarrow HgCl_2$ | 2.6E-18 | Ariya et al. (2002) |
| G10700 | TrGBrHg | $Hg + Br \rightarrow HgBr$ | 3.0E-13 | Donohoue et al. (2006) |
| G10701 | TrGBrHg | $HgBr + Br \rightarrow HgBr_2$ | 2.5E-10*(temp/298.)**(-0.57) | Goodsite et al. (2004) |
| G10702 | TrGBrHg | $Hg + Br_2 \rightarrow HgBr_2$ | 9.0E-17 | Ariya et al. (2002) |
| G10703 | TrGBrHg | $Hg + BrO \rightarrow HgO + Br$ | 1.0E-15 | Raofie and Ariya (2003) |
| G10704 | TrGBrHg | $HgBr + BrO \rightarrow BrHgOBr$ | 3.0E-12 | Calvert and Lindberg (2003) |
| G10705 | TrGBrClHg | $HgCl + BrO \rightarrow ClHgOBr$ | 3.0E-12 | Calvert and Lindberg (2003) |
| G10706 | TrGBrClHg | $HgBr + Cl \rightarrow ClHgBr$ | 3.0E-12 | Calvert and Lindberg (2003) |
| G10707 | TrGBrClHg | $HgCl + Br \rightarrow ClHgBr$ | 3.0E-12 | Calvert and Lindberg (2003) |

# General notes

## Three-body reactions

Rate coefficients for three-body reactions are defined via the function k_3rd($T$, $M$, $k_0^{300}$, $n$, $k_{\mathrm{inf}}^{300}$, $m$, $f_{\mathrm{c}}$). In the code, the temperature $T$ is called temp and the concentration of "air molecules" $M$ is called cair. Using the auxiliary variables $k_0(T)$, $k_{\mathrm{inf}}(T)$, and $k_{\mathrm{ratio}}$, k_3rd is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \tag{1}$$

$$k_{\mathrm{inf}}(T) = k_{\mathrm{inf}}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \tag{2}$$

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \tag{3}$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_{\mathrm{c}}^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}}))^2}\right)} \tag{4}$$

A similar function, called k_3rd_iupac here, is used by Wallington et al. (2018) for three-body reactions. It has the same function parameters as k_3rd and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \tag{5}$$

$$k_{\mathrm{inf}}(T) = k_{\mathrm{inf}}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \tag{6}$$

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \tag{7}$$

$$N = 0.75 - 1.27 \times \log_{10}(f_{\mathrm{c}}) \tag{8}$$

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_{\mathrm{c}}^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}})/N)^2}\right)} \tag{9}$$

## Structure-Activity Relationships (SAR)

Some unmeasured rate coefficients are estimated with structure-activity relationships, using the following parameters and substituent factors:

| $k$ for H-abstraction by OH in $\mathrm{cm^{-3}s^{-1}}$ | |
|---|---|
| k_p | $4.49 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-320\,\mathrm{K}/T)$ |
| k_s | $4.50 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(253\,\mathrm{K}/T)$ |
| k_t | $2.12 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(696\,\mathrm{K}/T)$ |
| k_ROHRO | $2.1 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-85\,\mathrm{K}/T)$ |
| k_CO2H | $0.7 \times k_{\mathrm{CH_3CO_2H+OH}}$ |
| k_ROOHRO | $0.6 \times k_{\mathrm{CH_3OOH+OH}}$ |
| f_alk | 1.23 |
| f_sOH | 3.44 |
| f_tOH | 2.68 |
| f_sOOH | 8. |
| f_tOOH | 8. |
| f_ONO2 | 0.04 |
| f_CH2ONO2 | 0.20 |
| f_cpan | 0.25 |
| f_allyl | 3.6 |
| f_CHO | 0.55 |
| f_CO2H | 1.67 |
| f_CO | 0.73 |
| f_O | 8.15 |
| f_pCH2OH | 1.29 |
| f_tCH2OH | 0.53 |

| $k$ for OH-addition to double bonds in $\mathrm{cm^{-3}s^{-1}}$ | |
|---|---|
| k_adp | $4.5 \times 10^{-12} \times (T/300\,\mathrm{K})^{-0.85}$ |
| k_ads | $1/4 \times (1.1 \times 10^{-11} \times \exp(485\,\mathrm{K}/T)+$ $1.0 \times 10^{-11} \times \exp(553\,\mathrm{K}/T))$ |
| k_adt | $1.922 \times 10^{-11} \times \exp(450\,\mathrm{K}/T) - k_{\mathrm{ads}}$ |
| k_adsecprim | $3.0 \times 10^{-11}$ |
| k_adtertprim | $5.7 \times 10^{-11}$ |
| a_PAN | 0.56 |
| a_CHO | 0.31 |
| a_COCH3 | 0.76 |
| a_CH2OH | 1.7 |
| a_CH2OOH | 1.7 |
| a_COH | 2.2 |
| a_COOH | 2.2 |
| a_CO2H | 0.25 |
| a_CH2ONO2 | 0.64 |

## $RO_2$ self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as decribed by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{1\mathrm{st}} = 2 \times \sqrt{k_{\mathrm{self}} \times \texttt{k\_CH3O2}} \times [\mathrm{RO_2}]$ where $k_{\mathrm{self}}$ = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH3O2 = second-order rate coefficient of the self reaction of $CH_3O_2$, and $[\mathrm{RO_2}]$ = sum of the concentrations of all organic peroxy radicals.

## Specific notes

G1002a: The path leading to 2 $O(^3P)$ + $O_2$ results in a null cycle regarding odd oxygen and is neglected.

G2110: The rate coefficient is: k_HO2_HO2 = (3.0E-13*EXP(460./temp)+2.1E-33*EXP(920./temp) *cair)*(1.+1.4E-21*EXP(2200./temp)*C(ind_H2O)).

G2117: Converted to Kc [molec-1 cm3]= Kp*R*T/NA, where R is 82.05736 [cm3atmK1mol1].

G2118: Assuming fast equilibrium.

G3109: The rate coefficient is: k_NO3_NO2 = k_3rd(temp,cair,2.4E-30,3.0,1.6E-12,-0.1,0.6).

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is: k_NO2_HO2 = k_3rd(temp,cair,1.9E-31,3.4,4.0E-12,0.3,0.6).

G3206: The rate coefficient is: k_HNO3_OH = 1.32E-14 * EXP(527/temp) + 1 / ( 1 / (7.39E-32 * EXP(453/temp)*cair) + 1 / (9.73E-17 * EXP(1910/temp)) )

G3207: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3227: Backward reaction divided by equilibrium constant from Burkholder et al. (2015).

G3228: Same as for OH + $HNO_4$.

G4104b: Methyl nitrate yield according to Banic et al. (2003) but reduced by a factor of 10 according to the upper limit derived from measurements by Munger et al. (1999).

G4109: Same temperature dependence as for $CH_3CHO$+$NO_3$ assumed.

G4115: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4116: Same value as for PAN + OH.

G4126: Same as for G4104 but scaled to match the recommeded value at 298K.

G4127: Same as for CH3O2 + NO3 in G4105.

G4130a: SAR for H-abstraction by OH.

G4130b: SAR for H-abstraction by OH.

G4132: SAR for H-abstraction by OH.

G4133: Lower limit of the rate constant. Products uncertain but $CH_3OH$ can be excluded because of a likely high energy barrier (L. Vereecken, pers. comm.). $CH_2OO$ production cannot be excluded.

G4134: Estimate based on the decomposition lifetime of 3 s (Olzmann et al., 1997) and a 20 kcal/mol energy barrier (Vereecken and Francisco, 2012).

G4135: Rate constant for $CH_2OO + NO_2$ (G4138) multiplied by the factor from Ouyang et al. (2013).

G4136: Average of two measurements.

G4137: Upper limit.

G4138: Average of 7.E-12 and 1.5E-12.

G4141: $HOOCH_2OCHO$ forms and then decomposes to formic anhydride (Gruzdev et al., 1993) which hydrolyses in the humid atmosphere (Conn et al., 1942).

G4142: High-pressure limit.

G4143: Generic estimate for reaction with alcohols.

G4144: Generic estimate for reaction with $RO_2$.

G4148: Same value as for $NO_2$+$CH_3O_2$.

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of $CH_3O_2NO_2$.

G4150: Value for $CH_3O_2NO_2$ + OH, H-abstraction enhanced by the HO-group by f_sOH.

G4154: Products assumed to be $CH_3O_2 + O_2$ (could also be $HCHO + O_2 + OH$).

G4160b: Half of the H-yield is attributed to fast secondary chemistry.

G4160c: The NH + CO channel is also significant but neglected here.

G4161: No studies below 450 K and only the major channel is considered.

G4164: Upper limit. Dominant pathway under atmospheric conditions.

G42001: The product distribution is from Rickard and Pascoe (2009), after substitution of the energized Criegee intermediate, $CH_2OO$, by its decomposition products and reaction of the stabilized CI with the water dimer.

G42010: Only major channel considered as the end products are essentially the same.

G42013: The rate coefficient is: k_CH3CO3_NO2 = k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6).

G42018: The rate coefficient is the same as for the $CH_3$ channel in G4107 ($CH_3OOH$+OH).

G42021: The rate coefficient is k_PAN_M = k_CH3CO3_NO2/9.0E-29*EXP(-14000./temp), i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G42022a: Quantum yields and products are from Glowacki et al. (2012).

G42022b: Quantum yields and products are from Glowacki et al. (2012).

G42024a: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42024b: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42047: Orlando et al. (1998) estimated that about 25% of the $HOCH_2CH_2O$ in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + $HO_2$.

G42051a: Same as for the $CH_3O_2$ channel in G4107: $CH_3OOH$+OH.

G42058b: The aldehydic H is assumed to be like the analogous H of $HOCH_2CHO$.

G42074a: Factor of 3 to match the estimate of k = 1.E-11 molec/cm3/s by Paulot et al. (2009a).

G42074b: Factor of 3 to match the estimate of k = 1.E-11 molec/cm3/s by Paulot et al. (2009a).

G42075: $NO_3CH_2CO_2H$ and $NO_3CH_2CO_3H$ neglected.

G42078: $NO_3CH_2CO_2H$ neglected.

G42082: Same rate constant as for PAN + OH.

G42083a: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42083b: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42085a: Uncertainties on the kinetics at pressures < 0.1 bar.

G42085b: Channel proposed by Hynes and Wine 1991, OH + HCHO + HOCN, could not be confirmed by Tyndall et al. (2001b). There is no alternative mechanism at the moment. Products assumed to be OH + CH3CO3 + NO

G42086b: Assuming HCN is from channel 2h, HCO + H + HCN. HCO is replaced by H + CO.

G42086c: Assuming exothermic channels 2b and 2d are equally important.

G42087: HCOCN is produced but replaced here by its likely oxidation products (HCN + $CO_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $RO_2$ + NO reaction is used.

G42088: $NCCH_2OOH$ is produced but replaced here by its likely oxidation products (HCN + $CO_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $RO_2$ + $HO_2$ reaction is used.

G42089a: The minor channel with k=5.2E-12 is combined with the major one producing HCOOH.

G42090: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G42091: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G42092: approximated OH reaction for oxalic acid

G42093a: SAR for H-abstraction by OH

G42093b: SAR for H-abstraction by OH, assuming that -CHOHOH has an effect like -CH2OH

G42093c: SAR for H-abstraction by OH

G42093d: SAR for H-abstraction by OH

G42094a: SAR for H-abstraction by OH

G42094b: SAR for H-abstraction by OH

G42095a: SAR for H-abstraction by OH

G42095b: SAR for H-abstraction by OH

G42096a: SAR for H-abstraction by OH

G42096b: SAR for H-abstraction by OH

G42097a: SAR for H-abstraction by OH

G42097b: SAR for H-abstraction by OH

G42098a: SAR for H-abstraction by OH, assuming that -CH2OOH has the same effect as -CH2OH

G42098b: SAR for H-abstraction by OH

G42098c: SAR for H-abstraction by OH

G43001a: Branching ratios according to Rickard et al. (1999).

G43001b: Branching ratios according to Rickard et al. (1999).

G43004: The value for the generic $RO_2$ + $HO_2$ reaction from Atkinson (1997) is used here.

G43008: The value for the generic $RO_2$ + $HO_2$ reaction from Atkinson (1997) is used here.

G43011: Strong positive deviation of k below 240 K compared to the expression recommended by JPL (Burkholder et al., 2015).

G43015a: The same value as for G4107 ($CH_3OOH$ + OH) is used, multiplied by the branching ratio of the $CH_3O_2$ channel.

G43028: Alkyl nitrate formation neglected. (also not considered in MCM).

G43037: Alkyl nitrate formation neglected. (also not considered in MCM).

G43040a: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43040b: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43044: Alkyl nitrate formation neglected.

G43045c: Rate coefficient assumed to equal to the one of hydroxyacetone (ACETOL) for this channel.

G43048: Using the high-pressure limit.

G43049: The pressure fall-off between 1000 and 100 mbar is only 3% (Kirchner et al., 1999).

G43050: Value for $CH_3O_2NO_2$ + OH, H-abstraction enhanced by the $CH_3CO$-group by f_CO.

G43051c: Products approximated with $C_2H_5CHO$ + $HO_2$.

G43052: Only major H-abstraction channel considered.

G43059: Products approximated with the major end-product $CH_3CHO$.

G43060b: Products approximated with the major end-product $CH_3CHO$.

G43061: Products approximated with the likely end-product $CH_3CHO$.

G43065: As for $HCOCO_3$.

G43070a: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43070b: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43071a: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G43072: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G43073: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G43074: HCOCOCHO would be produced but undergoes fast photolysis (faster than MGLYOX) and is substituted with its products.

G43075a: Same value as for methanediol.

G43075b: Same value as for methanediol.

G43223: Products simplified

G43419: KDEC C3DIALO → GLYOX + CO + HO2

G43420: KDEC C3DIALO → GLYOX + CO + HO2

G43421: Permutation reaction (minor channels removed).

G44000: The $LC_4H_9O_2$ composition ($nC_4H_9O_2$:$sC_4H_9O_2$ ratio) is assumed to be equal to the ratio of the production rates at 298K: k_p/(k_p+k_s) = 0.1273 and k_s/(k_p+k_s) = 0.8727.

G44001b: $sC_4H_9O_2$ products are substituted with 0.636 MEK + $HO_2$ and 0.364 $CH_3CHO$ + $C_2H_5O_2$ at 1 bar and 298 K.

G44003c: The alkyl nitrate yield is the weighted average yield for the two isomers forming from $nC_4H_9O_2$ and $sC_4H_9O_2$.

G44010b: H-abstraction from primary C and substitution of the resulting peroxy radical with its products from the reaction with NO.

G44011: H-abstraction from primary C and substitution of the resulting peroxy radical with its products from the reaction with NO.

G44015b: Products assumed to be only from H-abstraction from a secondary C bearing the -OOH group.

G44016: Products assumed to be only from H-abstraction from a secondary C bearing the $-ONO_2$ group.

G44018: LHMVKABO2 is 0.12 HMVKAO2 + 0.88 HMVKBO2.

G44019: LMEKO2 represents 0.62 MEKBO2 + 0.38 MEKAO2.

G44021a: The products of MEKAO are substituted with HCHO + $CO_2$ + $HOCH_2CH_2O_2$.

G44023a: Products from H-abstraction from the tertiary carbon bearing the $ONO_2$ group.

G44023b: Products from H-abstraction from the secondary carbon bearing the $ONO_2$ group.

G44025: Same value as for PAN.

G44026: Products as in G4415. Only the main channels for each isomer are considered. Weighted average for the isomers.

G44035: Rate constant replaced with the one of beta hydroxy $RO_2$.

G44046b: Using value for secondary nitrate (88% of total).

G44061a: Using value for secondary nitrate (88% of total).

G44061b: Using value for secondary nitrate (88% of total).

G44062a: Simplified products.

G44062b: Simplified products.

G44066: Alkyl nitrate formation neglected.

G44070: Alkyl nitrate formation neglected.

G44076: Alkyl nitrate formation neglected.

G44078: Other channel neglected.

G44081: Alkyl nitrate formation neglected.

G44082: Other channel neglected.

G44085: k for $CH_3CHCO$ from Hatakeyama et al. (1985) adjusted.

G44086: Simplified product distribution.

G44089: The nitrated $RO_2$ is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO2 isomers mostly $C_2H_5CHO$.

G44097a: Branching ratios according to Rickard et al. (1999). $CH_3CHO_2CHO$ is replaced with its major products $CH_3CHO$ + CO + $HO_2$.

G44097b: Branching ratios according to Rickard et al. (1999).

G44098: The nitrated $RO_2$ is replaced by its products upon reaction with NO.

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH3CHOOA products as from $C_3H_6$ + $O_3$ reaction.

G44107: The nitrated $RO_2$ is replaced by its products upon reaction with NO.

G44110: The nitrated $RO_2$ is replaced by its products upon reaction with NO.

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

G44127: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G44128: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44129: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44130: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G44131: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44132: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44133: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G44134: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44135: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44136: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G44137: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44138: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44139: Simplified oxidation.

G44140: Simplified oxidation.

G44141: Simplified oxidation.

G44142: Simplified oxidation.

G44202: Alkyl nitrate formation neglected.

G44203a: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G44205: Alkyl nitrate formation neglected.

G44210: Alkyl nitrate formation neglected.

G44221: Same k as for MGLYOX + OH (Tyndall et al., 1995).

G44402: KDEC NC4DCO2→ MALANHY + NO2

G44406c: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44407: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44409: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44410: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44412: KDEC BZFUONOOA → 0.5 BZFUONOO + 0.5 CO + 0.5 CO2 + 0.5 HCOCH2O2 + 0.5 OH and BZFUONOO → 0.625 CO14O3CO2H + 0.375 CO14O3CHO + 0.375 H2O2

G44421: Only major channel.

G44424: KDEC: GLYOOA → 0.125 HCHO + 0.18 GLYOO + 0.82 HO2 + 0.57 OH + 1.265 CO + 0.25 CO2 and H2O substitution GLYOO → 0.625 HCOCO2H + 0.375 GLYOX + 0.375 H2O2

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCO3

G44431: KDEC MALANHYO → HCOCOHCO3

G44432: Only major channel. KDEC MALANHYO → HCOCOHCO3

G44436: KDEC NBZFUO → 0.5 CO14O3CHO + 0.5 NO2 + 0.5 NBZFUONE + 0.5 HO2

G44437: KDEC NBZFUO → 0.5 CO14O3CHO + 0.5 NO2 + 0.5 NBZFUONE + 0.5 HO2

G44438: KDEC NBZFUO → 0.5 CO14O3CHO + 0.5 NO2 + 0.5 NBZFUONE + 0.5 HO2 and RO2 Only major channel.

G44439: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44443: KDEC MECOACETO → CH3CO3 + HCHO

G44444: KDEC MECOACETO → CH3CO3 + HCHO

G44445: KDEC MECOACETO → CH3CO3 + HCHO

G44450: KDEC BZFUO → CO14O3CHO + HO2

G44451: KDEC BZFUO → CO14O3CHO + HO2

G44452: KDEC BZFUO → CO14O3CHO + HO2. Only major channel.

G44457: KDEC MALDIALO → GLYOX + GLYOX + HO2

G44458: KDEC MALDIALO → GLYOX + GLYOX + HO2

G44459: KDEC MALDIALO → GLYOX + GLYOX + HO2. Only major channel.

G44461: KBPAN → k_PAN_M

G45019d: Delta-1 and delta-2 LIEPOX are not considered and replaced by beta-LIEPOX formed by ISOPBOOH and ISOPDOOH.

G45021: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 1.1E-11.

G45037: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 4.2E-11.

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant 4.16E-11.

G45047: Alkyl nitrate formation neglected.

G45055: Alkyl nitrate formation neglected.

G45071: Alkyl nitrate formation neglected.

G45074: Formic acid production consistent with results of Bates et al. (2014). Here, the high yields of formic acid and hydroxycarbonyls at low NO from oxidation of cis-beta-LIEPOX (the most abundant isomer) are approximated with the production of DB1O which undergo both the Dibble double H-transfer to DB2O2 and HOCH2 elimination yielding HVMK and HMAC (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting from the ring opening after H-abstraction). The rate constant is from Paulot et al. (2009b) and adjusted based on Bates et al. (2014) that determined the single rate constants for the cis- and trans- beta isomer.

G45080: Alkyl nitrate formation neglected.

G45092a: C4MDIAL = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with $NO_3$ but only one isomer product considered.

G45095: Alkyl nitrate formation neglected.

G45098: Alkyl nitrate formation neglected.

G45100: Alkyl nitrate formation neglected.

G45104a: DB1OOH is a hydroperoxide bearing a vinyl alcohol moiety that upon reaction with OH yields HCOOH (Davis et al., 1998).

G45107: OH production here is to take into account the hydroperoxidic function formed by the shift of the enolic hydrogen and not present in DB2O2. This approximation leads to spurious $HO_2$ production.

G45108a: Consistent with the results of Bates et al. (2014).

G45108b: Consistent with the results of Bates et al. (2014). Assuming that the enol alkoxy radical partly decomposes yielding a substitute vinyl alcohol.

G45111: Alkyl nitrate formation neglected.

G45114b: Here, formic acid is mechanistically produced by the OH-addition to the vinyl alcohol which, upon $RO_2$-to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with $O_2$ forming $HCOOH + HO_2$. Along $CH_3COCHOOHCHO$ should be produced but not in the mechanism. Only $CH_3COCHO_2CHO$. The rate constant is consistent with predictions by Ganzeveld et al. (2006) for ENOL. OH-addition to the OH-bearing carbon is considered the dominant channel as it is already for the ENOL (Ganzeveld et al., 2006).

G45115: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006). The product should be C1ODC3OOHC4OD but it is neglected in the mechanism.

G45116: As for DB1OOH + OH.

G45117: Additional sinks for DB2OOH are neglected.

G45121b: Nitrate assumed to be major isomer that is mostly similar to products of ISOPDO2-chemistry.

G45128: Rate constant by Liljegren and Stevens (2013). A lumped $RO_2$ that upon conversion to RO yields 100% 2-methyl-butenedial (C4MDIAL) although Aschmann et al. (2014) quantified a 38% yield of the Z/E mixture.

G45129: As for 3METHYLFURAN + OH but with additional $NO_2$ production for mass conservation.

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

G45134b: ZCO2HC23DBCOD formation is neglected. However, it is produced in MCM and in aromatic-related reactions under the name of MC3ODBCO2H.

G45139: LZCPANC23DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO2 = 0.67 MBOAO2 + 0.33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2 → MMALANHY + NO2

G45404: KDEC NTLFUO → ACCOMECHO + NO2

G45405: KDEC NTLFUO → ACCOMECHO + NO2

G45406: KDEC NTLFUO → ACCOMECHO

G45409: KBPAN → k_PAN_M(renaming)

G45413: KFPAN → k_CH3CO3_NO2 (renaming)

G45422: KDEC MMALANHYO→CO2H3CO3

G45423: KDEC MMALANHYO→CO2H3CO3

G45424: KDEC MMALANHYO→CO2H3CO3 and Only major channel.

G45429: KBPAN → k_PAN_M (renamed)

G45430a: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + 0.17 MGLYOX + 0.17 HO2 + 0.17 CO + 0.17 CO2

G45431: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + 0.17 MGLYOX + 0.17 HO2 + 0.17 CO + 0.17 CO2

G45432: KFPAN →k_CH3CO3_NO2 (renaming)

G45433: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + 0.17 MGLYOX + 0.17 HO2 + 0.17 CO + 0.17 CO2

G45434: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + 0.17 MGLYOX + 0.17 HO2 + 0.17 CO + 0.17 CO2 and only major channel.

G45436: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + 0.17 MGLYOX + 0.17 HO2 + 0.17 CO + 0.17 CO2

G45444: KDEC MC3CODBCO2 → 0.35 GLYOX + 0.35 CH3 + 0.35 CO + 0.35 CO2 + 0.65 MMALANHY + 0.65 HO2

G45452: KDEC TLFUONOOA → 0.5 CO + 0.5 OH + 0.5 MECOACETO2 + 0.5 TLFUONOO and H2O subs TLFUONOO → 0.625 C24O3CCO2H + 0.375 ACCOMECHO + 0.375 H2O2

G45456: KFPAN →k_CH3CO3_NO2 (renaming)

G45476b: KDEC NTLFUO → ACCOMECHO + NO2 and reactions with KRO2HO2.

G45477: KDEC NTLFUO → ACCOMECHO + NO2

G45478: KDEC NTLFUO → ACCOMECHO + NO2

G45479: KDEC NTLFUO → ACCOMECHO + NO2

G45486b: KDEC C5DIALO →MALDIAL + CO + HO2 and reactions with KRO2HO2.

G45487: KDEC C5DIALO →MALDIAL

G45488: KDEC C5DIALO →MALDIAL

G45489: KDEC C5DIALO →MALDIAL

G45491b: Reactions with KRO2HO2.

G45492: MGLYOX + GLYOX + HO2 from KDEC substitution

G45493: MGLYOX + GLYOX + HO2 from KDEC substitution

G45494: Permutation reaction (minor channels removed).

G46201: Alkyl nitrate formation neglected.

G46404b: Reactions with KRO2HO2 and KDEC C615CO2O → C5DICARB + CO + HO2.

G46405: KDEC C615CO2O → C5DICARB + CO + HO2

G46406: KDEC C615CO2O → C5DICARB + CO + HO2

G46407: Only major channel.

G46413b: Reactions with KRO2HO2 and KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2.

G46414: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46415: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46416: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46418: KDEC CATECOOA → MALDALCO2H + HCOCO2H + HO2 + OH

G46426: KFPAN →k_CH3CO3_NO2

G46430: KDEC GLYOOA → .125 HCHO + .18 GLYOO + .82 HO2 + .57 OH + 1.265 CO

G46432b: Reactions with KRO2HO2 and KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46433: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46434: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46435: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46437b: Reactions with KRO2HO2 and KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46438: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46439: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46440: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46441: Merged equations.

G46447b: reactions with KRO2HO2 and KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46448: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46449: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46450: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46457: Merged equations.

G46458: Merged equations.

G46461b: Reactions with KRO2HO2 and KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46462: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46463: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46464: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2 and Only major channel.

G46468: KFPAN →k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO →C5CO2OHCO3

G46481: KDEC PBZQO →C5CO2OHCO3

G46482: KDEC PBZQO →C5CO2OHCO3

G46483: KDEC PBZQO →C5CO2OHCO3 and Only major channel.

G46485b: Reactions with KRO2HO2 and KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46486: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46490b: Reactions with KRO2HO2 and KDEC BZEMUCO → 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO.

G46491b: KDEC BZEMUCO → 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO.

G46492: KDEC BZEMUCO → 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO

G46493: KDEC BZEMUCO → 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO and Only major channel.

G46499b: Reactions with KRO2HO2 and KDEC NBZQO → C6CO4DB + NO2.

G46500: KDEC NBZQO → C6CO4DB + NO2

G46501: KDEC NBZQO → C6CO4DB + NO2

G46502: KDEC NBZQO → C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

G46522b: In analogy to TLBIPERO2 from toluene (Birdsall et al., 2010).

G46523b: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46524: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46525: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE and Only major channel.

G47210: Alkyl nitrate formation neglected.

G47214: Alkyl nitrate formation neglected.

G47218: Alkyl nitrate formation neglected.

G47222: Alkyl nitrate formation neglected.

G47223: ROO6R3OOH produced but no sink for it.

G47225: ROO6R4P produced but no sink for it.

G47226: ROO6R5P produced but no sink for it

G47400: Merged.

G47402a: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47402b: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47403: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47404: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2. C6H5CH2OH replaced by its oxidation product BENZAL.

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero2_oh is set to 0.4 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

G47408a: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 C4MDIAL + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47408b: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47409: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47410: Only major channel and KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47412: KDEC MGLOOB → 0.125 CH3CHO + 0.695 CH3CO + 0.57 CO + 0.57 OH + 0.125 HO2 + 0.18 MGLOO + 0.25 CO2

G47413: Merged.

G47418b: Reactions with KRO2HO2 and KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE.

G47419: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

G47420: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

G47421: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE and Only major channel.

G47422b: Reactions with KRO2HO2 and KDEC NCRESO → C5CO14OH + GLYOX + NO2

G47423: KDEC NCRESO → C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO → C5CO14OH + GLYOX + NO2

G47425: KDEC NCRESO → C5CO14OH + GLYOX + NO2 and Only major channel.

G47426: TOL1OHNO2 is a nitro-phenol

G47429: KDEC MCATECOOA → MC3ODBCO2H + HCOCO2H + HO2 + OH

G47436: KFPAN →k_CH3CO3_NO2

G47438: Only major channel.

G47439b: Reactions with KRO2HO2 and KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47440b: KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47441: KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47442: KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2 and Only major channel.

G47445: KFPAN →k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

G47482b: Reactions with KRO2HO2 and KDEC NPTLQO → C7CO4DB + NO2

G47483: KDEC NPTLQO → C7CO4DB + NO2

G47484: KDEC NPTLQO → C7CO4DB + NO2

G47485: KDEC NPTLQO → C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO → C6CO2OHCO3

G47487: KDEC PTLQO → C6CO2OHCO3

G47488: KDEC PTLQO → C6CO2OHCO3

G47489: Only major channel. KDEC PTLQO → C6CO2OHCO3.

G47494: New channel.

G47497b: Reactions with KRO2HO2 and KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47498: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47501b: Reactions with KRO2HO2 and KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47502: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47509b: Reactions with KRO2HO2 and KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47510: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47511: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47512: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47513b: Reactions with KRO2HO2 and KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47514: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G48202: Alkyl nitrate formation neglected.

G48205: Alkyl nitrate formation neglected.

G48210: Alkyl nitrate formation neglected.

G48212: Alkyl nitrate formation neglected.

G48216: Alkyl nitrate formation neglected.

G48222: Alkyl nitrate formation neglected.

G48400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (1.36E-11*0.24 + 2.31E-11*0.29 + 1.43E-11*0.155)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400b: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (1.36E-11*0.05 + 2.31E-11*0.04 + 1.43E-11*0.10)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (1.36E-11*0.16 + 2.31E-11*0.17 + 1.43E-11*0.12)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400d: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (1.36E-11*0.55 + 2.31E-11*0.50 + 1.43E-11*0.625)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48401: Same products as for toluene. The rate constant is the average of m, p, o k=(4.10E-16+2.60E-16+5.00E-16)/3 = 3.9E-16.

G48402: merged under same rate constant

G48403: Same products as for toluene

G48405: KDEC CH2OOB → 0.24 CH2OO + 0.40 CO + 0.36 HO2 + 0.36 CO + 0.36 OH and H2O + PHCHOO → 0.625 PHCOOH + 0.375 BENZAL + 0.375 H2O2 + 0.2 CO2

G48408: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

G48409: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

G48410: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

G48412b: KDEC STYRENO → HO2 + HCHO + BENZAL and reactions with KRO2HO2.

G48413: KDEC STYRENO → HO2 + HCHO + BENZAL

G48414: KDEC STYRENO → HO2 + HCHO + BENZAL

G48415: KDEC STYRENO → HO2 + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

G49246: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.Instead of the (lacking) carbonyl a product of further degradation is assumed.

G49247: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G49248: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (3.27E-11*0.21 + 3.25E-11*0.30 + 5.67E-11*0.14)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400b: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (3.27E-11*0.06 + 3.25E-11*0.06 + 5.67E-11*0.03)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (3.27E-11*0.03 + 3.25E-11*0.03 + 5.67E-11*.04)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400d: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (3.27E-11*0.70 + 3.25E-11*0.61 + 5.67E-11*0.79)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49401: Same products as for toluene. The rate constant is the average of m, p, o k=(1.90+1.80+0.88)E-15/3=1.52E-15.

G40200: Products from Vereecken et al. (2007). LAPINABO2 = 0.65 APINAO2 + 0.35 APINBO2

G40203: Weighted average for isomers A and B, `k = 0.33*9.20E-14+0.67*8.80E-13`.

G40204: Weighted average for isomers A and B, `k = 0.35*1.83E-11+0.65*3.28E-11`.

G40205: Weighted average for isomers A and B, `k = 0.35*5.50E-12+0.65*3.64E-12`.

G40206: SAR-estimated rate constant, `(kads+kadt)*acoch3 = 6.46E-11` where `kads = 3.0E-11`, `kadt = 5.5E-11`, `acoch3 = 0.76`

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard and Pascoe (2009).

G40212: Products from Rickard and Pascoe (2009).

G40232: Products from Capouet et al. (2008).

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard and Pascoe (2009).

G40248: Alkyl nitrate formation neglected.

G40252a: Products from Vereecken and Peeters (2012).

G40252b: Products from Vereecken and Peeters (2012).

G40259: ROO6R1OOH is produced but no sink for it.

G40262: RO6R1OOH is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

G40267a: Products from Nguyen et al. (2009).

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for RO6R1NO3 in G4085.

G40276: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.

G40277: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G40278: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G40282a: Products from Vereecken and Peeters (2012).

G40282b: Products from Vereecken and Peeters (2012).

G40283a: Products from Nguyen et al. (2009).

G40284: Products from Rickard and Pascoe (2009).

G40285a: Products from Vereecken and Peeters (2012).

G40285b: Products from Vereecken and Peeters (2012).

G40286a: Products from Nguyen et al. (2009).

G40287: Products from Rickard and Pascoe (2009).

G40400: DIET35TOL(from MCM) as representative of higher aromatics

G40401: Same products as for toluene.

G6103: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G6204: At low temperatures, there may be a minor reaction channel leading to $O_3$+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

G6402: The initial products are probably HCl and $CH_2OOH$ (Atkinson et al., 2006). It is assumed that $CH_2OOH$ dissociates into HCHO and OH.

G6409: It is assumed that the reaction liberates all Cl atoms in the form of HCl.

G7302: The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

G7303: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (Orlando and Tyndall, 1996).

G7404: It is assumed that the reaction liberates all Br atoms in the form of HBr.

G7407: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7408: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7605: Same value as for G7408: $CH_2Br_2$+OH assumed. It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

G7606: Same value as for G7408: $CH_2Br_2$+OH assumed. It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

G7607: It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

G8102: Consistent with O'Dowd and Hoffmann (2005), it is assumed that the reaction produces new particles.

G8103: The yield of 38 % OIO is from Atkinson et al. (2007). It is assumed here that the remaining 62 % produce 2 I + $O_2$.

G8300: The rate coefficient is: `k_I_NO2 = k_3rd_iupac(temp,cair,3.E-31,1.,6.6E-11,0.,0.63)`.

G8305: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (van den Bergh and Troe, 1976).

G8401: The rate coefficient is from Dillon et al. (2006b), the yield of I atoms is a lower limit given on page 2170 of Bale et al. (2005).

G8402: The products are from Nakano et al. (2005).

G8701: 80% Br + OIO production is from Atkinson et al. (2007). The remaining channels are assumed to produce Br + I + $O_2$.

G9400a: For the abstraction path, the assumed reaction sequence (omitting $H_2O$ and $O_2$ as products) according to Yin et al. (1990) is:

$$
\begin{array}{rcl}
\mathrm{DMS + OH} & \rightarrow & \mathrm{CH_3SCH_2} \\
\mathrm{CH_3SCH_2 + O_2} & \rightarrow & \mathrm{CH_3SCH_2OO} \\
\mathrm{CH_3SCH_2OO + NO} & \rightarrow & \mathrm{CH_3SCH_2O + NO_2} \\
\mathrm{CH_3SCH_2O} & \rightarrow & \mathrm{CH_3S + HCHO} \\
\mathrm{CH_3S + O_3} & \rightarrow & \mathrm{CH_3SO} \\
\mathrm{CH_3SO + O_3} & \rightarrow & \mathrm{CH_3SO_2} \\
\hline
\mathrm{DMS + OH + NO + 2O_3} & \rightarrow & \mathrm{CH_3SO_2 + HCHO + NO_2}
\end{array}
$$

Neglecting the effect on $O_3$ and $NO_x$, the remaining reaction is:

$$\mathrm{DMS + OH + O_3 \rightarrow CH_3SO_2 + HCHO}$$

.

G9400b: For the addition path, the rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

G9402: Products and yields are not from Hynes and Wine (1996).

G9408: Average of 3.9E-11 and 3.42E-11.

G10201: Upper limit.

Table 2: Photolysis reactions

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J (gas) | | | | |
| J0001 | UpGJ | $O(^3P) \rightarrow O^+ + e^-$ | jx(ip_Op_em) +jx(ip_se_Op_em) | Fuller-Rowell (1993) |
| J0002a | UpGJ | $O_2 \rightarrow O_2^+ + e^-$ | jx(ip_O2p_em) +jx(ip_se_O2_b1) | Fuller-Rowell (1993) |
| J0002b | UpGJ | $O_2 \rightarrow O^+ + O(^3P) + e^-$ | jx(ip_Op_O_em) +jx(ip_se_O2_b2) | Fuller-Rowell (1993) |
| J0003a | UpGJN | $N_2 \rightarrow N_2^+ + e^-$ | jx(ip_N2p_em) +jx(ip_se_N2_b1) | Fuller-Rowell (1993) |
| J0003b | UpGJN | $N_2 \rightarrow N^+ + N + e^-$ | jx(ip_Np_N_em) +jx(ip_se_N2_b2) | Fuller-Rowell (1993) |
| J0003c | UpGJN | $N_2 \rightarrow N^+ + N(^2D) + e^-$ | jx(ip_Np_N2D_em)+jx(ip_se_N2_b3) | Fuller-Rowell (1993) |
| J0003d | UpGJN | $N_2 \rightarrow N + N(^2D)$ | jx(ip_N_N2D_em) +jx(ip_se_N2_b4) | Fuller-Rowell (1993) |
| J1000a | UpStTrGJ | $O_2 + h\nu \rightarrow O(^3P) + O(^3P)$ | jx(ip_O2) | Sander et al. (2014) |
| J1000b | UpGJ | $O_2 + h\nu \rightarrow O(^3P) + O(^1D)$ | jx(ip_O3PO1D) | Sander et al. (2014) |
| J1000c | UpGJ | $O_2 + h\nu \rightarrow O_2^+ + e^-$ | jx(ip_O2_b1) | Sander et al. (2014) |
| J1000d | UpGJ | $O_2 + h\nu \rightarrow O^+ + O(^3P) + e^-$ | jx(ip_O2_b2) | Sander et al. (2014) |
| J1001a | UpStTrGJ | $O_3 + h\nu \rightarrow O(^1D) + O_2$ | jx(ip_O1D) | Sander et al. (2014) |
| J1001b | UpStTrGJ | $O_3 + h\nu \rightarrow O(^3P) + O_2$ | jx(ip_O3P) | Sander et al. (2014) |
| J1002 | UpGJ | $O(^3P) + h\nu \rightarrow O^+ + e^-$ | jx(ip_O3Pp) | Sander et al. (2014) |
| J2100a | UpStGJ | $H_2O + h\nu \rightarrow H + OH$ | jx(ip_H2O) | Sander et al. (2014) |
| J2100b | UpGJ | $H_2O + h\nu \rightarrow H_2 + O(^1D)$ | jx(ip_H2O1D) | Sander et al. (2014) |
| J2101 | UpStTrGJ | $H_2O_2 + h\nu \rightarrow 2\ OH$ | jx(ip_H2O2) | Sander et al. (2014) |
| J3000a | UpGJN | $N_2 + h\nu \rightarrow N_2^+ + e^-$ | jx(ip_N2_b1) | Sander et al. (2014) |
| J3000b | UpGJN | $N_2 + h\nu \rightarrow N^+ + N + e^-$ | jx(ip_N2_b2) | Sander et al. (2014) |
| J3000c | UpGJN | $N_2 + h\nu \rightarrow N^+ + N(^2D) + e^-$ | jx(ip_N2_b3) | Sander et al. (2014) |
| J3000d | UpGJN | $N_2 + h\nu \rightarrow N + N(^2D)$ | jx(ip_NN2D) | Sander et al. (2014) |
| J3100 | UpStGJN | $N_2O + h\nu \rightarrow O(^1D) + N_2$ | jx(ip_N2O) | Sander et al. (2014) |
| J3101 | UpStTrGJN | $NO_2 + h\nu \rightarrow NO + O(^3P)$ | jx(ip_NO2) | Sander et al. (2014) |
| J3102a | UpStGJN | $NO + h\nu \rightarrow N + O(^3P)$ | jx(ip_NO) | Sander et al. (2014) |
| J3102b | UpGJN | $NO + h\nu \rightarrow NO^+ + e^-$ | jx(ip_NOp) | Sander et al. (2014) |
| J3103a | UpStTrGJN | $NO_3 + h\nu \rightarrow NO_2 + O(^3P)$ | jx(ip_NO2O) | Sander et al. (2014) |
| J3103b | UpStTrGJN | $NO_3 + h\nu \rightarrow NO + O_2$ | jx(ip_NOO2) | Sander et al. (2014) |
| J3104 | StTrGJN | $N_2O_5 + h\nu \rightarrow NO_2 + NO_3$ | jx(ip_N2O5) | Sander et al. (2014) |
| J3200 | TrGJN | $HONO + h\nu \rightarrow NO + OH$ | jx(ip_HONO) | Sander et al. (2014) |
| J3201 | StTrGJN | $HNO_3 + h\nu \rightarrow NO_2 + OH$ | jx(ip_HNO3) | Sander et al. (2014) |
| J3202 | StTrGJN | $HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$ | jx(ip_HNO4) | Sander et al. (2014) |
| J41000 | StTrGJ | $CH_3OOH + h\nu \rightarrow CH_3O + OH$ | jx(ip_CH3OOH) | Sander et al. (2014) |
| J41001a | StTrGJ | $HCHO + h\nu \rightarrow H_2 + CO$ | jx(ip_COH2) | Sander et al. (2014) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J41001b | StTrGJ | $HCHO + h\nu \rightarrow H + CO + HO_2$ | `jx(ip_CHOH)` | Sander et al. (2014) |
| J41002 | StGJ | $CO_2 + h\nu \rightarrow CO + O(^3P)$ | `jx(ip_CO2)` | Sander et al. (2014) |
| J41003 | StGJ | $CH_4 + h\nu \rightarrow .42\ CH_3 + .42\ H + .6912\ H_2 + .0864\ HCHO + .0864\ O(^3P) + .1584\ OH + .1584\ HO_2 + .2112\ CO_2 + .1824\ CO + .024\ H_2O + .10\ LCARBON$ | `jx(ip_CH4)` | Sander et al. (2014)* |
| J41004 | StTrGJN | $CH_3ONO + h\nu \rightarrow CH_3O + NO$ | `jx(ip_CH3ONO)` | Sander et al. (2014) |
| J41005 | StTrGJN | $CH_3ONO_2 + h\nu \rightarrow CH_3O + NO_2$ | `jx(ip_CH3NO3)` | Sander et al. (2014) |
| J41006 | StTrGJN | $CH_3O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ CH_3O_2 + .333\ NO_3 + .333\ CH_3O$ | `jx(ip_CH3O2NO2)` | Sander et al. (2014)* |
| J41007 | StTrGJ | $HOCH_2OOH + h\nu \rightarrow HCOOH + OH + HO_2$ | `jx(ip_CH3OOH)` | Sander et al. (2014) |
| J41008 | StTrGJ | $CH_3O_2 + h\nu \rightarrow HCHO + OH$ | `jx(ip_CH3O2)` | Sander et al. (2014) |
| J41009 | StTrGJ | $HCOOH + h\nu \rightarrow CO + HO_2 + OH$ | `jx(ip_HCOOH)` | Sander et al. (2014) |
| J41010 | StTrGJN | $HOCH_2O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ HOCH_2O_2 + .333\ NO_3 + .333\ HCOOH + .333\ HO_2$ | `jx(ip_CH3O2NO2)` | Sander et al. (2014) |
| J42000 | TrGJC | $C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$ | `jx(ip_CH3OOH)` | von Kuhlmann (2001) |
| J42001a | TrGJC | $CH_3CHO + h\nu \rightarrow CH_3 + HO_2 + CO$ | `jx(ip_CH3CHO)` | Sander et al. (2014) |
| J42001b | TrGJC | $CH_3CHO + h\nu \rightarrow CH_2CHOH$ | `jx(ip_CH3CHO2VINY)` | Clubb et al. (2012) |
| J42002 | TrGJC | $CH_3C(O)OOH + h\nu \rightarrow CH_3 + OH + CO_2$ | `jx(ip_CH3CO3H)` | Sander et al. (2014) |
| J42004 | TrGJCN | $PAN + h\nu \rightarrow .7\ CH_3C(O) + .7\ NO_2 + .3\ CH_3 + .3\ CO_2 + .3\ NO_3$ | `jx(ip_PAN)` | Sander et al. (2014)* |
| J42005a | TrGJC | $HOCH_2CHO + h\nu \rightarrow HCHO + 2\ HO_2 + CO$ | `jx(ip_HOCH2CHO)*0.83` | Sander et al. (2014)* |
| J42005b | TrGJC | $HOCH_2CHO + h\nu \rightarrow OH + HCOCH_2O_2$ | `jx(ip_HOCH2CHO)*0.07` | Sander et al. (2014)* |
| J42005c | TrGJC | $HOCH_2CHO + h\nu \rightarrow CH_3OH + CO$ | `jx(ip_HOCH2CHO)*0.10` | Sander et al. (2014)* |
| J42006 | TrGJC | $HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$ | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J42007 | TrGJCN | $PHAN + h\nu \rightarrow .7\ HOCH2CO + .7\ NO_2 + .3\ HCHO + .3\ HO_2 + .3\ CO_2 + .3\ NO_3$ | `jx(ip_PAN)` | see note* |
| J42008 | TrGJC | $GLYOX + h\nu \rightarrow 2\ CO + 2\ HO_2$ | `jx(ip_GLYOX)` | Sander et al. (2014) |
| J42009 | TrGJC | $HCOCO_2H + h\nu \rightarrow 2\ HO_2 + CO + CO_2$ | `jx(ip_MGLYOX)` | Rickard and Pascoe (2009) |
| J42010 | TrGJC | $HCOCO_3H + h\nu \rightarrow HO_2 + CO + OH + CO_2$ | `jx(ip_CH3OOH)+jx(ip_HOCH2CHO)` | Rickard and Pascoe (2009) |
| J42011 | TrGJC | $HYETHO2H + h\nu \rightarrow HOCH_2CH_2O + OH$ | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J42012 | TrGJCN | $ETHOHNO3 + h\nu \rightarrow HO_2 + 2\ HCHO + NO_2$ | `j_IC3H7NO3` | Rickard and Pascoe (2009) |
| J42013 | TrGJC | $HOOCH2CO3H + h\nu \rightarrow OH + HCHO + CO_2 + OH$ | `2.*jx(ip_CH3OOH)` | Sander et al. (2019) |
| J42014 | TrGC | $HOOCH2CO2H + h\nu \rightarrow OH + HCHO + HO_2 + CO_2$ | `jx(ip_CH3OOH)` | Sander et al. (2019) |
| J42015 | TrGC | $CH2CO + h\nu \rightarrow .4\ CO_2 + .8\ H + .34\ CO + .34\ OH + .34\ HO_2 + .16\ HCHO + .16\ O(^3P) + .1\ HCOOH + CO$ | `j_ketene*0.36` | Sander et al. (2019) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J42016 | TrGC | CH3CHOHOOH + h$\nu$ $\rightarrow$ $CH_3$ + HCOOH + OH | `jx(ip_CH3OOH)` | Sander et al. (2019) |
| J42017 | TrGJCN | $NO_3$CH2CHO + h$\nu$ $\rightarrow$ $HO_2$ + CO + HCHO + $NO_2$ | `(jx(ip_C2H5NO3)+jx(ip_CH3CHO))*(jx(ip_NOA)+1E-10)/(0.59*j_IC3H7NO3+jx(ip_CH3COCH3)+1E-10)` | Sander et al. (2019)* |
| J42018 | TrGJC | HOOCH2CHO + h$\nu$ $\rightarrow$ OH + HCHO + CO + $HO_2$ | `jx(ip_CH3OOH)+jx(ip_HOCH2CHO)` | Sander et al. (2019) |
| J42019 | TrGJCN | $C_2H_5ONO_2$ + h$\nu$ $\rightarrow$ $CH_3CHO$ + $HO_2$ + $NO_2$ | `jx(ip_C2H5NO3)` | Sander et al. (2019) |
| J42020 | TrGJCN | $NO_3$CH2CHO + h$\nu$ $\rightarrow$ .7 $NO_3$CH2$CO_3$ + .7 $NO_2$ + .3 HCHO + .3 $NO_2$ + .3 $CO_2$ + .3 $NO_3$ | `jx(ip_PAN)` | Sander et al. (2019)* |
| J42021 | StTrGJCN | $C_2H_5O_2NO_2$ + h$\nu$ $\rightarrow$ .667 $NO_2$ + .667 $C_2H_5O_2$ + .333 $NO_3$ + .333 $CH_3CHO$ + .333 $HO_2$ | `jx(ip_CH3O2NO2)` | Sander et al. (2019)* |
| J42022 | TrGJC | HOOCCOOH + h$\nu$ $\rightarrow$ $CO_2$ + .72 HCOOH + .28 CO + .28 $H_2O$ | `jx(ip_HOOCCOOH)` | Yamamoto and Back (1985) |
| J43000 | TrGJC | i$C_3H_7OOH$ + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $HO_2$ + OH | `jx(ip_CH3OOH)` | von Kuhlmann (2001) |
| J43001 | TrGJC | $CH_3COCH_3$ + h$\nu$ $\rightarrow$ $CH_3C(O)$ + $CH_3$ | `jx(ip_CH3COCH3)` | Sander et al. (2014) |
| J43002 | TrGJC | $CH_3COCH_2OH$ + h$\nu$ $\rightarrow$ .5 $CH_3C(O)$ + .5 HCHO + .5 $HO_2$ + .5 HOCH2CO + .5 $CH_3$ | `j_ACETOL` | Sander et al. (2014)* |
| J43003 | TrGJC | MGLYOX + h$\nu$ $\rightarrow$ $CH_3C(O)$ + CO + $HO_2$ | `jx(ip_MGLYOX)` | Sander et al. (2014) |
| J43004 | TrGJC | $CH_3COCH_2O_2H$ + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCHO + OH | `jx(ip_CH3OOH)+j_ACETOL` | Rickard and Pascoe (2009) |
| J43005 | TrGJC | HOCH2COCH2OOH + h$\nu$ $\rightarrow$ HOCH2CO + HCHO + OH | `jx(ip_CH3OOH)+j_ACETOL` | Sander et al. (2019) |
| J43006 | TrGJCN | i$C_3H_7ONO_2$ + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $NO_2$ + $HO_2$ | `j_IC3H7NO3` | von Kuhlmann et al. (2003)* |
| J43007 | TrGJCN | NOA + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCHO + $NO_2$ | `jx(ip_NOA)` | Barnes et al. (1993) |
| J43009 | TrGJC | HYPROPO2H + h$\nu$ $\rightarrow$ $CH_3CHO$ + HCHO + $HO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J43010 | TrGJCN | PR2O2HNO3 + h$\nu$ $\rightarrow$ NOA + $HO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J43011 | TrGJC | HOCH2COCHO + h$\nu$ $\rightarrow$ HOCH2CO + CO + $HO_2$ | `jx(ip_MGLYOX)` | Rickard and Pascoe (2009) |
| J43012 | TrGJC | $HCOCOCH_2OOH$ + h$\nu$ $\rightarrow$ HCOCO + HCHO + OH | `jx(ip_CH3OOH)+j_ACETOL` | Sander et al. (2019) |
| J43013 | TrGJC | $HCOCOCH_2OOH$ + h$\nu$ $\rightarrow$ $HOOCH_2CO_3$ + CO + $HO_2$ | `jx(ip_MGLYOX)` | Sander et al. (2019) |
| J43014 | TrGJTerC | HCOCH2CHO + h$\nu$ $\rightarrow$ $HCOCH_2O_2$ + $HO_2$ + CO | `jx(ip_HOCH2CHO)*2.` | Rickard and Pascoe (2009) |
| J43015 | TrGJTerC | HCOCH2CO2H + h$\nu$ $\rightarrow$ $HCOCH_2O_2$ + $CO_2$ + $HO_2$ | `jx(ip_HOCH2CHO)` | Rickard and Pascoe (2009) |
| J43016 | TrGJTerC | HOC2H4CO3H + h$\nu$ $\rightarrow$ $HOCH_2CH_2O_2$ + $CO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J43017 | TrGJC | HCOCOCHO + h$\nu$ $\rightarrow$ HCOCO + $HO_2$ + CO | `2.*jx(ip_MGLYOX)` | Sander et al. (2019) |
| J43018 | TrGJC | $CH_3COCO_2H$ + h$\nu$ $\rightarrow$ .32 $CH_3CHO$ + .16 $CH_2CHOH$ + .54 $CO_2$ + .38 $CH_3C(O)$ + .38 $HO_2$ + .38 $CO_2$ + .07 $CH_3COOH$ + .07 CO + .05 $CH_3C(O)$ + .05 CO + .05 OH | `jx(ip_CH3COCO2H)` | Sander et al. (2019)* |
| J43019 | TrGC | $CH_3COCO_3H$ + h$\nu$ $\rightarrow$ $CH_3C(O)$ + OH + $CO_2$ | `jx(ip_MGLYOX)+jx(ip_CH3OOH)` | Sander et al. (2019) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J43020 | TrGC | CH3CHCO + h$\nu$ $\rightarrow$ $C_2H_4$ + CO | j_ketene*0.36*2. | Sander et al. (2019) |
| J43021 | TrGCN | PROPOLNO3 + h$\nu$ $\rightarrow$ $HOCH_2CHO$ + HCHO + $HO_2$ + $NO_2$ | j_IC3H7NO3 | Sander et al. (2019) |
| J43022 | TrGCN | $CH_3COCH_2OONO_2$ + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCHO + $NO_3$ | jx(ip_CH3O2NO2)+jx(ip_CH3COCH3) | Sander et al. (2019) |
| J43023 | TrGJC | $C_3H_7OOH$ + h$\nu$ $\rightarrow$ $C_2H_5CHO$ + $HO_2$ + OH | jx(ip_CH3OOH) | von Kuhlmann (2001) |
| J43024 | TrGJCN | $C_3H_7ONO_2$ + h$\nu$ $\rightarrow$ $C_2H_5CHO$ + $NO_2$ + $HO_2$ | 0.59*j_IC3H7NO3 | see note* |
| J43025a | TrGJC | $C_2H_5CHO$ + h$\nu$ $\rightarrow$ $C_2H_5O_2$ + $HO_2$ + CO | jx(ip_C2H5CHO2HCO) | see note* |
| J43025b | TrGJC | $C_2H_5CHO$ + h$\nu$ $\rightarrow$ $CH_2CHCH_2OH$ | jx(ip_C2H5CHO2ENOL) | Andrews et al. (2012), Sander et al. (2019)* |
| J43026 | TrGJCN | PPN + h$\nu$ $\rightarrow$ .7 $C_2H_5CO_3$ + .7 $NO_2$ + .3 $C_2H_5O_2$ + .3 $CO_2$ + .3 $NO_3$ | jx(ip_PAN) | Sander et al. (2014) |
| J43027 | TrGJC | $C_2H_5CO_3H$ + h$\nu$ $\rightarrow$ $C_2H_5O_2$ + $CO_2$ + OH | jx(ip_CH3OOH) | von Kuhlmann (2001) |
| J43028a | TrGJC | $HCOCOCH_2OOH$ + h$\nu$ $\rightarrow$ $HOOCH_2CO_3$ + CO + $HO_2$ | jx(ip_MGLYOX) | Sander et al. (2019) |
| J43028b | TrGJC | $HCOCOCH_2OOH$ + h$\nu$ $\rightarrow$ HCOCO + HCHO + OH | jx(ip_HOCH2CHO)+jx(ip_CH3OOH) | Sander et al. (2019) |
| J43200 | TrGJTerC | HCOCH2CO3H + h$\nu$ $\rightarrow$ $HCOCH_2O_2$ + $CO_2$ + OH | jx(ip_HOCH2CHO)+jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J43400 | TrGJAroC | C3DIALOOH + h$\nu$ $\rightarrow$ GLYOX + CO + $HO_2$ + OH | jx(ip_HOCH2CHO)*2.+jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J43401 | TrGJAroC | C32OH13CO + h$\nu$ $\rightarrow$ GLYOX + $HO_2$ + $HO_2$ + CO | jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J43402 | TrGJAroC | HCOCOHCO3H + h$\nu$ $\rightarrow$ GLYOX + $HO_2$ + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J44000a | TrGJC | $LC_4H_9OOH$ + h$\nu$ $\rightarrow$ OH + $C_3H_7CHO$ + $HO_2$ | jx(ip_CH3OOH)*(k_p/(k_p+k_s)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| J44000b | TrGJC | $LC_4H_9OOH$ + h$\nu$ $\rightarrow$ OH + .636 MEK + .636 $HO_2$ + .364 $CH_3CHO$ + .364 $C_2H_5O_2$ | jx(ip_CH3OOH)*(k_s/(k_p+k_s)) | Rickard and Pascoe (2009), Sander et al. (2019) |
| J44001 | TrGJC | MVK + h$\nu$ $\rightarrow$ .5 $C_3H_6$ + .5 $CH_3C(O)$ + .5 HCHO + CO + .5 $HO_2$ | jx(ip_MVK) | Sander et al. (2014) |
| J44002 | TrGJC | MEK + h$\nu$ $\rightarrow$ $CH_3C(O)$ + $C_2H_5O_2$ | 0.42*jx(ip_CHOH) | von Kuhlmann et al. (2003) |
| J44003 | TrGJC | LMEKOOH + h$\nu$ $\rightarrow$ .62 $CH_3C(O)$ + .62 $CH_3CHO$ + .38 HCHO + .38 $CO_2$ + .38 $HOCH_2CH_2O_2$ + OH | jx(ip_CH3OOH)+0.42*jx(ip_CHOH) | Sander et al. (2019) |
| J44004 | TrGJC | BIACET + h$\nu$ $\rightarrow$ 2 $CH_3C(O)$ | 2.15*jx(ip_MGLYOX) | see note* |
| J44005a | TrGJCN | LC4H9NO3 + h$\nu$ $\rightarrow$ $NO_2$ + $C_3H_7CHO$ + $HO_2$ | j_IC3H7NO3*(k_p/(k_p+k_s)) | see note* |
| J44005b | TrGJCN | LC4H9NO3 + h$\nu$ $\rightarrow$ $NO_2$ + MEK + $HO_2$ | j_IC3H7NO3*(k_s/(k_p+k_s)) | see note* |
| J44006 | TrGJCN | MPAN + h$\nu$ $\rightarrow$ .7 MACO3 + .7 $NO_2$ + .3 MACO2 + .3 $NO_3$ | jx(ip_PAN) | see note* |
| J44007a | TrGJC | CO2H3CO3H + h$\nu$ $\rightarrow$ MGLYOX + $HO_2$ + OH + $CO_2$ | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J44007b | TrGJC | CO2H3CO3H + h$\nu$ → $CH_3C(O)$ + $HO_2$ + $HCOCO_3H$ | j_ACETOL | Rickard and Pascoe (2009) |
| J44008 | TrGJC | MACR + h$\nu$ → .5 MACO3 + .5 $CH_3C(O)$ + .5 HCHO + .5 CO + $HO_2$ | jx(ip_MACR) | Sander et al. (2014) |
| J44009 | TrGJC | MACROOH + h$\nu$ → MACRO + OH | jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO) | Sander et al. (2019)* |
| J44010 | TrGJC | MACROH + h$\nu$ → $CH_3COCH_2OH$ + CO + $HO_2$ + $HO_2$ | 2.77*jx(ip_HOCH2CHO) | see note* |
| J44011 | TrGJC | MACO3H + h$\nu$ → MACO2 + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44012 | TrGJC | LHMVKABOOH + h$\nu$ → .12 MGLYOX + .12 $HO_2$ + .88 $CH_3C(O)$ + .88 $HOCH_2CHO$ + .12 HCHO + OH | jx(ip_CH3OOH)+j_ACETOL | Sander et al. (2019) |
| J44013 | TrGJC | CO2H3CHO + h$\nu$ → MGLYOX + CO + $HO_2$ + $HO_2$ | jx(ip_HOCH2CHO)+j_ACETOL | Sander et al. (2019) |
| J44014 | TrGJC | HO12CO3C4 + h$\nu$ → $CH_3C(O)$ + $HOCH_2CHO$ + $HO_2$ | j_ACETOL | Rickard and Pascoe (2009) |
| J44015 | TrGJC | BIACETOH + h$\nu$ → $CH_3C(O)$ + HOCH2CO | 2.15*jx(ip_MGLYOX) | see note* |
| J44016 | TrGC | $HCOCCH_3CO$ + h$\nu$ → .5 OH + .5 $CH_3CHO$ + CO + .5 CH3CHCO + .5 CO | j_ketene | Sander et al. (2019) |
| J44017a | TrGC | $CH_3COCHCO$ + h$\nu$ → .0192 $CH_3COCO_2H$ + .1848 $H_2O_2$ + .2208 MGLYOX + .36 OH + .36 CO + .56 $CH_3C(O)$ + .2 $CH_3CHO$ + .2 $CO_2$ + .2 HCHO + .2 $HO_2$ + CO | j_ketene*0.5 | Sander et al. (2019),Rickard and Pascoe (2009)* |
| J44017b | TrGC | $CH_3COCHCO$ + h$\nu$ → CH3CHCO + CO | j_ketene*0.5 | Sander et al. (2019) |
| J44018a | TrGJC | $CH_3COCOCHO$ + h$\nu$ → $CH_3C(O)$ + 2 CO + $HO_2$ | jx(ip_MGLYOX) | Sander et al. (2019) |
| J44018b | TrGJC | $CH_3COCOCHO$ + h$\nu$ → HCOCO + $CH_3C(O)$ | 2.15*jx(ip_MGLYOX) | Sander et al. (2019) |
| J44019 | TrGJC | CH3COCOCO2H + h$\nu$ → $CH_3C(O)$ + CO + $CO_2$ + $HO_2$ | 3.15*jx(ip_MGLYOX) | Sander et al. (2019) |
| J44020a | TrGJTerC | $CH_3COCOCH_2OOH$ + h$\nu$ → $CH_3C(O)$ + OH + HCHO + CO | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |
| J44020b | TrGJTerC | $CH_3COCOCH_2OOH$ + h$\nu$ → $CH_3C(O)$ + HCOCO | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J44021 | TrGJTerC | C44OOH + h$\nu$ → HCOCH2CHO + $CO_2$ + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J44022 | TrGJTerC | C413COOOH + h$\nu$ → HCOCH2CO3 + HCHO + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO)+j_ACETOL | Rickard and Pascoe (2009) |
| J44023a | TrGJTerC | C4CODIAL + h$\nu$ → $HCOCOCH_2O_2$ + $HO_2$ + CO | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J44023b | TrGJTerC | C4CODIAL + h$\nu$ → HCOCH2CO3 + $HO_2$ + CO | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J44024 | TrGJTerC | C312COCO3H + h$\nu$ → $HCOCOCH_2O_2$ + $CO_2$ + OH | jx(ip_CH3OOH)+jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J44025 | TrGJCN | LMEKNO3 + h$\nu$ → .62 $CH_3C(O)$ + .62 $CH_3CHO$ + .38 HCHO + .38 $CO_2$ + .38 $HOCH_2CH_2O_2$ + $NO_2$ | jx(ip_MEKNO3) | Barnes et al. (1993), Sander et al. (2019)* |
| J44026 | TrGJCN | MVKNO3 + h$\nu$ → $CH_3C(O)$ + $HOCH_2CHO$ + $NO_2$ | jx(ip_MEKNO3) | Barnes et al. (1993), Sander et al. (2019)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J44027 | TrGJCN | MACRNO3 + h$\nu$ $\rightarrow$ $CH_3COCH_2OH$ + CO + $HO_2$ + $NO_2$ | (2.84*j_IC3H7NO3+jx(ip_CH3CHO)) *(jx(ip_MEKNO3)+1E-10)/(j_ IC3H7NO3+0.42*jx(ip_CHOH)+1E-10) | Müller et al. (2014), Sander et al. (2019)* |
| J44028 | TrGJCN | TC4H9NO3 + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $CH_3$ + $NO_2$ | 2.84*j_IC3H7NO3 | Sander et al. (2019) |
| J44029 | TrGJC | $TC_4H_9OOH$ + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $CH_3$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44030 | TrGJCN | IBUTOLBNO3 + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + HCHO + $HO_2$ + $NO_2$ | 2.84*j_IC3H7NO3 | Sander et al. (2019) |
| J44031 | TrGJC | IBUTOLBOOH + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + HCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44032 | TrGJC | LBUT1ENOOH + h$\nu$ $\rightarrow$ $C_2H_5CHO$ + HCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44033 | TrGJCN | LBUT1ENNO3 + h$\nu$ $\rightarrow$ $C_2H_5CHO$ + HCHO + $HO_2$ + $NO_2$ | j_IC3H7NO3 | Sander et al. (2019) |
| J44034 | TrGJC | BUT2OLOOH + h$\nu$ $\rightarrow$ 2 $CH_3CHO$ + $HO_2$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44035 | TrGJCN | BUT2OLNO3 + h$\nu$ $\rightarrow$ 2 $CH_3CHO$ + $HO_2$ + $NO_2$ | j_IC3H7NO3 | Sander et al. (2019) |
| J44036 | TrGJC | BUT2OLO + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HOCH2CO | j_ACETOL | Sander et al. (2019) |
| J44037a | TrGJC | $C_3H_7CHO$ + h$\nu$ $\rightarrow$ $C_3H_7O_2$ + CO + $HO_2$ | jx(ip_C3H7CHO2HCO) | Sander et al. (2019) |
| J44037b | TrGJC | $C_3H_7CHO$ + h$\nu$ $\rightarrow$ $C_2H_4$ + $CH_2CHOH$ | jx(ip_C3H7CHO2VINY) | Sander et al. (2019)* |
| J44038 | TrGJC | IPRCHO + h$\nu$ $\rightarrow$ $iC_3H_7O_2$ + CO + $HO_2$ | jx(ip_IPRCHO2HCO) | Sander et al. (2019) |
| J44039 | TrGJCN | IC4H9NO3 + h$\nu$ $\rightarrow$ IPRCHO + $NO_2$ | j_IC3H7NO3 | Sander et al. (2019) |
| J44040 | TrGJC | $IC_4H_9OOH$ + h$\nu$ $\rightarrow$ IPRCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44041 | TrGJC | PERIBUACID + h$\nu$ $\rightarrow$ $iC_3H_7O_2$ + $CO_2$ + OH | jx(ip_CH3OOH) | Sander et al. (2019) |
| J44042 | TrGJCN | PIPN + h$\nu$ $\rightarrow$ .7 IPRCO3 + .7 $NO_2$ + .3 $iC_3H_7O_2$ + .3 $CO_2$ + .3 $NO_3$ | jx(ip_PAN) | Sander et al. (2019), Sander et al. (2014) |
| J44043 | TrGJC | HVMK + h$\nu$ $\rightarrow$ MGLYOX + CO + 2 OH | jx(ip_PeDIONE24) | Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)* |
| J44044 | TrGJC | HMAC + h$\nu$ $\rightarrow$ $HCOCCH_3CO$ + 2 OH | jx(ip_PeDIONE24) | Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)* |
| J44045a | TrGJC | CO2C3CHO + h$\nu$ $\rightarrow$ $CH_3COCH_2O_2$ + $HO_2$ + CO | jx(ip_C2H5CHO2HCO) | Rickard and Pascoe (2009) |
| J44045b | TrGJC | CO2C3CHO + h$\nu$ $\rightarrow$ HVMK | jx(ip_C2H5CHO2ENOL) | Andrews et al. (2012), Sander et al. (2019) |
| J44046a | TrGJC | IBUTDIAL + h$\nu$ $\rightarrow$ $CH_3CHO$ + CO + $HO_2$ + $CO_2$ + $H_2O$ | jx(ip_C2H5CHO2HCO)*2. | see note* |
| J44046b | TrGJC | IBUTDIAL + h$\nu$ $\rightarrow$ HMAC | jx(ip_C2H5CHO2ENOL)*2. | Andrews et al. (2012), Sander et al. (2019) |
| J44200 | TrGJTerC | IBUTALOH + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $HO_2$ + $HO_2$ + CO | j_ACETOL | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J44201 | TrGJTerC | IPRHOCO3H + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + $HO_2$ + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J44400a | TrGJAroC | MALDIALOOH + h$\nu$ $\rightarrow$ C32OH13CO + CO + OH + $HO_2$ | jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J44400b | TrGJAroC | MALDIALOOH + h$\nu$ $\rightarrow$ GLYOX + GLYOX + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J44401 | TrGJAroC | BZFUOOH + h$\nu$ $\rightarrow$ CO14O3CHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J44402 | TrGJAroC | HOCOC4DIAL + h$\nu$ $\rightarrow$ HCOCOHCO3 + $HO_2$ + CO | jx(ip_MGLYOX)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J44403 | TrGJAroCN | NBZFUOOH + h$\nu$ $\rightarrow$ .5 CO14O3CHO + .5 $NO_2$ + .5 NBZFUONE + .5 $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J44404a | TrGJAroC | MALDALCO3H + h$\nu$ $\rightarrow$ $HCOCO_3H$ + $HO_2$ + CO + $HO_2$ + CO | jx(ip_MACR) | Rickard and Pascoe (2009) |
| J44404b | TrGJAroC | MALDALCO3H + h$\nu$ $\rightarrow$ .6 MALANHY + $HO_2$ + .4 GLYOX + .4 CO + .4 $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J44405 | TrGJAroC | EPXDLCO2H + h$\nu$ $\rightarrow$ C3DIALO2 + $CO_2$ + $HO_2$ | 2.77*jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J44406 | TrGJAroC | MALDIAL + h$\nu$ $\rightarrow$ .4 BZFUONE + .6 MALDIALCO3 + .6 $HO_2$ | jx(ip_NO2)*0.14 | Rickard and Pascoe (2009) |
| J44407 | TrGJAroC | MALANHYOOH + h$\nu$ $\rightarrow$ HCOCOHCO3 + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J44408 | TrGJAroC | EPXDLCO3H + h$\nu$ $\rightarrow$ C3DIALO2 + OH + $CO_2$ | jx(ip_CH3OOH)+2.77*jx(ip_ HOCH2CHO) | Rickard and Pascoe (2009) |
| J44409 | TrGJAroC | CO2C4DIAL + h$\nu$ $\rightarrow$ CO + CO + $HO_2$ + $HO_2$ + CO + CO | jx(ip_MGLYOX)*2. | Rickard and Pascoe (2009) |
| J44410 | TrGJAroC | MALDALCO2H + h$\nu$ $\rightarrow$ $HCOCO_2H$ + $HO_2$ + CO + $HO_2$ + CO | jx(ip_MACR) | Rickard and Pascoe (2009) |
| J44411 | TrGJAroC | EPXC4DIAL + h$\nu$ $\rightarrow$ C3DIALO2 + CO + $HO_2$ | 2.77*jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J44412 | TrGJAroC | CO14O3CHO + h$\nu$ $\rightarrow$ $HO_2$ + CO + $HCOCH_2O_2$ + $CO_2$ | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J44414 | TrGJAroC | MECOACEOOH + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCHO + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J45002 | TrGJC | LISOPACOOH + h$\nu$ $\rightarrow$ LISOPACO + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J45003 | TrGJCN | LISOPACNO3 + h$\nu$ $\rightarrow$ LISOPACO + $NO_2$ | 0.59*j_IC3H7NO3 | see note* |
| J45004 | TrGJC | ISOPBOOH + h$\nu$ $\rightarrow$ MVK + HCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J45005 | TrGJCN | ISOPBNO3 + h$\nu$ $\rightarrow$ MVK + HCHO + $HO_2$ + $NO_2$ | 2.84*j_IC3H7NO3 | see note* |
| J45006 | TrGJC | ISOPDOOH + h$\nu$ $\rightarrow$ MACR + HCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J45007 | TrGJCN | ISOPDNO3 + h$\nu$ $\rightarrow$ MACR + HCHO + $HO_2$ + $NO_2$ | j_IC3H7NO3 | see note* |
| J45008 | TrGJCN | NISOPOOH + h$\nu$ $\rightarrow$ NC4CHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J45009 | TrGJCN | NC4CHO + h$\nu$ $\rightarrow$ LHC4ACCO3 + $NO_2$ | (.59*j_IC3H7NO3+jx(ip_MACR)) *(jx(ip_MEKNO3)+1E-10)/(j_ IC3H7NO3+0.42*jx(ip_CHOH)+1E-10) | Müller et al. (2014), Sander et al. (2019)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J45010 | TrGJCN | LNISOOH + h$\nu$ $\rightarrow$ NOA + OH + .5 HOCHCHO + .5 CO + .5 $HO_2$ + .5 $CO_2$ | jx(ip_CH3OOH) | Taraborrelli et al. (2009), Sander et al. (2019) |
| J45011 | TrGJC | LHC4ACCHO + h$\nu$ $\rightarrow$ .5 LHC4ACCO3 + .5 $HO_2$ + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2 | jx(ip_MACR) | Sander et al. (2019) |
| J45012 | TrGJC | LC578OOH + h$\nu$ $\rightarrow$ .25 $CH_3COCH_2OH$ + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 $HO_2$ + OH | jx(ip_CH3OOH)+ 2.77*jx(ip_HOCH2CHO) | Sander et al. (2019) |
| J45013 | TrGJC | LHC4ACCO3H + h$\nu$ $\rightarrow$ OH + .5 MACRO2 + .5 LHMVKABO2 + OH + $CO_2$ | j_HPALD | Sander et al. (2019) |
| J45014 | TrGJCN | LC5PAN1719 + h$\nu$ $\rightarrow$ .7 LHC4ACCO3 + .7 $NO_2$ + .15 MACRO2 + .15 LHMVKABO2 + .3 $CO_2$ + .3 $NO_3$ | jx(ip_PAN) | Sander et al. (2019) |
| J45015 | TrGJC | HCOC5 + h$\nu$ $\rightarrow$ .65 $CH_3$ + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + HOCH2CO | 0.5*jx(ip_MVK) | Sander et al. (2019)* |
| J45016 | TrGJC | C59OOH + h$\nu$ $\rightarrow$ $CH_3COCH_2OH$ + HOCH2CO + OH | j_ACETOL+jx(ip_CH3OOH) | Sander et al. (2019) |
| J45017 | TrGJTerC | C511OOH + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCOCH2CHO + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45018a | TrGJTerC | CO23C4CHO + h$\nu$ $\rightarrow$ $CH_3COCOCH_2O_2$ + $HO_2$ + CO | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45018b | TrGJTerC | CO23C4CHO + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCOCH2CO3 | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45019 | TrGJTerC | CO23C4CO3H + h$\nu$ $\rightarrow$ $CH_3COCOCH_2O_2$ + $CO_2$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45020 | TrGJTerC | C512OOH + h$\nu$ $\rightarrow$ C513O2 + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45021 | TrGJTerC | CO13C4CHO + h$\nu$ $\rightarrow$ CHOC3COO2 + CO + $HO_2$ | jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J45022 | TrGJTerC | C513OOH + h$\nu$ $\rightarrow$ GLYOX + $HOC_2H_4CO_3$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45023 | TrGJTerC | C513CO + h$\nu$ $\rightarrow$ $HOC_2H_4CO_3$ + $HO_2$ + CO + CO | jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45024 | TrGJTerC | C514OOH + h$\nu$ $\rightarrow$ CO13C4CHO + $HO_2$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J45025 | TrGJTerCN | C514NO3 + h$\nu$ $\rightarrow$ CO13C4CHO + $HO_2$ + $NO_2$ | j_IC3H7NO3+jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J45026a | TrGJC | LZCODC23DBCOOH + h$\nu$ $\rightarrow$ OH + CO + HVMK + OH | j_HPALD*0.6*0.5 | Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026b | TrGJC | LZCODC23DBCOOH + h$\nu$ $\rightarrow$ OH + CO + $CH_3C(O)$ + $HOCH_2CHO$ | j_HPALD*0.6*0.5 | Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026c | TrGJC | LZCODC23DBCOOH + h$\nu$ $\rightarrow$ OH + CO + HMAC + OH | j_HPALD*0.4*0.5 | Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026d | TrGJC | LZCODC23DBCOOH + h$\nu$ $\rightarrow$ OH + CO + CO + $CH_3COCH_2OH$ + $HO_2$ | j_HPALD*0.4*0.5 | Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J45027 | TrGJC | LZCO3HC23DBCOD + h$\nu$ $\rightarrow$ .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + $CO_2$ | `j_HPALD` | Sander et al. (2019) |
| J45028a | TrGJC | C1OOHC2OOHC4OD + h$\nu$ $\rightarrow$ $CH_3COCH_2O_2H$ + OH + 2 CO + $HO_2$ | `2.77*jx(ip_HOCH2CHO)` | Sander et al. (2019) |
| J45028b | TrGJC | C1OOHC2OOHC4OD + h$\nu$ $\rightarrow$ .5 $CH_3COCH_2O_2H$ + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH | `2.*jx(ip_CH3OOH)` | Sander et al. (2019) |
| J45029 | TrGC | DB1OOH + h$\nu$ $\rightarrow$ DB1O2 + OH | `jx(ip_CH3OOH)` | Sander et al. (2019) |
| J45030 | TrGC | DB2OOH + h$\nu$ $\rightarrow$ .48 $CH_3COCH_2OH$ + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + $HO_2$ + OH | `jx(ip_CH3OOH)` | Sander et al. (2019) |
| J45031a | TrGJC | C1ODC2OOHC4OD + h$\nu$ $\rightarrow$ MGLYOX + HOCHCHO + OH | `jx(ip_CH3OOH)` | Sander et al. (2019) |
| J45031b | TrGJC | C1ODC2OOHC4OD + h$\nu$ $\rightarrow$ CO2H3CHO + CO + $HO_2$ + OH | `2.*2.77*jx(ip_HOCH2CHO)` | Sander et al. (2019) |
| J45032 | TrGJC | C4MDIAL + h$\nu$ $\rightarrow$ .5 $CH_3COCHCO$ + .5 $HCOCCH_3CO$ + CO + $HO_2$ + OH | `jx(ip_NO2)*0.1*0.5` | Sander et al. (2019)* |
| J45033 | TrGCN | DB1NO3 + h$\nu$ $\rightarrow$ DB1O2 + $NO_2$ | `j_IC3H7NO3` | Sander et al. (2019) |
| J45034 | TrGJTerC | CHOC3COOOH + h$\nu$ $\rightarrow$ CHOC3COO2 + $CO_2$ + OH | `jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +j_ACETOL` | Rickard and Pascoe (2009) |
| J45200a | TrGJTerC | LMBOABOOH + h$\nu$ $\rightarrow$ $HOCH_2CHO$ + $CH_3COCH_3$ + $HO_2$ + OH | `jx(ip_CH3OOH)*.67` | Rickard and Pascoe (2009), Sander et al. (2019) |
| J45200b | TrGJTerC | LMBOABOOH + h$\nu$ $\rightarrow$ IBUTALOH + HCHO + $HO_2$ + OH | `jx(ip_CH3OOH)*.33` | Rickard and Pascoe (2009), Sander et al. (2019) |
| J45201 | TrGJTerC | MBOACO + h$\nu$ $\rightarrow$ HCHO + $HO_2$ + IPRHOCO3 | `j_ACETOL` | Rickard and Pascoe (2009) |
| J45202 | TrGJTerC | MBOCOCO + h$\nu$ $\rightarrow$ CO + $HO_2$ + IPRHOCO3 | `jx(ip_MGLYOX)` | Rickard and Pascoe (2009) |
| J45203a | TrGJTerCN | LNMBOABOOH + h$\nu$ $\rightarrow$ $NO_3CH2CHO$ + $CH_3COCH_3$ + $HO_2$ + OH | `jx(ip_CH3OOH)*.65` | Rickard and Pascoe (2009), Sander et al. (2019) |
| J45203b | TrGJTerCN | LNMBOABOOH + h$\nu$ $\rightarrow$ IBUTALOH + HCHO + $NO_2$ + OH | `jx(ip_CH3OOH)*.35` | Rickard and Pascoe (2009), Sander et al. (2019) |
| J45204 | TrGJTerCN | NC4OHCO3H + h$\nu$ $\rightarrow$ IBUTALOH + $CO_2$ + $NO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J45400 | TrGJAroC | C54CO + h$\nu$ $\rightarrow$ $HO_2$ + CO + CO + CO + $CH_3C(O)$ | `jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX) *2.` | Rickard and Pascoe (2009) |
| J45401 | TrGJAroC | C5134CO2OH + h$\nu$ $\rightarrow$ $CH_3COCOCHO$ + $HO_2$ + CO + $HO_2$ | `jx(ip_HOCH2CHO)+2.15*jx(ip_ MGLYOX)` | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J45402 | TrGJAroC | C5DIALOOH + h$\nu$ $\rightarrow$ MALDIAL + CO + $HO_2$ + OH | jx(ip_CH3OOH)+jx(ip_MACR) | Rickard and Pascoe (2009)* |
| J45406 | TrGJAroC | C5CO14OH + h$\nu$ $\rightarrow$ $CH_3C(O)$ + $HCOCO_2H$ + $HO_2$ + CO | jx(ip_MVK) | Rickard and Pascoe (2009) |
| J45407 | TrGJAroC | C5DICARB + h$\nu$ $\rightarrow$ .6 C5CO14O2 + .6 $HO_2$ + .4 TLFUONE | jx(ip_NO2)*0.2 | Rickard and Pascoe (2009)* |
| J45408 | TrGJAroC | MC3ODBCO2H + h$\nu$ $\rightarrow$ $CH_3COCO_2H$ + $HO_2$ + CO + $HO_2$ + CO | jx(ip_MACR) | Rickard and Pascoe (2009) |
| J45409 | TrGJAroC | ACCOMECHO + h$\nu$ $\rightarrow$ MECOACETO2 + $HO_2$ + CO | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45410 | TrGJAroC | MMALNHYOOH + h$\nu$ $\rightarrow$ CO2H3CO3 + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J45411 | TrGJAroC | C5DICAROOH + h$\nu$ $\rightarrow$ MGLYOX + GLYOX + $HO_2$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +j_ACETOL | Rickard and Pascoe (2009)* |
| J45412 | TrGJAroCN | NTLFUOOH + h$\nu$ $\rightarrow$ ACCOMECHO + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J45414 | TrGJAroC | C5CO14OOH + h$\nu$ $\rightarrow$ .83 MALANHY + .83 $CH_3$ + .17 MGLYOX + .17 $HO_2$ + .17 CO + .17 $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J45415 | TrGJAroC | TLFUOOH + h$\nu$ $\rightarrow$ ACCOMECHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J45417 | TrGJAroC | ACCOMECO3H + h$\nu$ $\rightarrow$ MECOACETO2 + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J45418 | TrGJAroC | C5DIALCO + h$\nu$ $\rightarrow$ MALDIALCO3 + CO + $HO_2$ | jx(ip_MGLYOX)+jx(ip_MACR) | Rickard and Pascoe (2009) |
| J46200 | TrGJTerCN | C614NO3 + h$\nu$ $\rightarrow$ CO23C4CHO + HCHO + $HO_2$ + $NO_2$ | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46201 | TrGJTerC | C614OOH + h$\nu$ $\rightarrow$ CO23C4CHO + HCHO + $HO_2$ + OH | jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46202 | TrGJTerC | CO235C5CHO + h$\nu$ $\rightarrow$ CO23C4CO3 + CO + $HO_2$ | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46203 | TrGJTerC | CO235C6OOH + h$\nu$ $\rightarrow$ CO23C4CO3 + HCHO + OH | jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46400 | TrGJAroC | PHENOOH + h$\nu$ $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46401 | TrGJAroC | C6CO4DB + h$\nu$ $\rightarrow$ C4CO2DBCO3 + $HO_2$ + CO | jx(ip_MGLYOX)*2. | Rickard and Pascoe (2009) |
| J46402 | TrGJAroC | C5CO2DCO3H + h$\nu$ $\rightarrow$ $CH_3C(O)$ + HCOCOCHO + $CO_2$ + OH | jx(ip_CH3OOH)+jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46403 | TrGJAroCN | NDNPHENOOH + h$\nu$ $\rightarrow$ NC4DCO2H + $HNO_3$ + CO + CO + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46404 | TrGJAroCN | BZBIPERNO3 + h$\nu$ $\rightarrow$ GLYOX + $HO_2$ + .5 BZFUONE + .5 BZFUONE + $NO_2$ | j_IC3H7NO3 | Rickard and Pascoe (2009)* |
| J46405 | TrGJAroCN | HOC6H4NO2 + h$\nu$ $\rightarrow$ HONO + CPDKETENE | jx(ip_HOC6H4NO2) | Chen et al. (2011)* |
| J46406 | TrGJAroC | CPDKETENE + h$\nu$ $\rightarrow$ $CO_2$ + CO + 2 $HO_2$ + MALDIAL | j_ketene | see note* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J46407 | TrGJAroC | C5COOHCO3H + h$\nu$ $\rightarrow$ HOCOC4DIAL + $HO_2$ + CO + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46408 | TrGJAroC | BZEPOXMUC + h$\nu$ $\rightarrow$ .5 C5DIALO2 + 1.5 $HO_2$ + 1.5 CO + .5 MALDIAL | 4.E3*jx(ip_MVK)*0.1 | Rickard and Pascoe (2009) |
| J46409 | TrGJAroCN | NPHEN1OOH + h$\nu$ $\rightarrow$ NPHEN1O + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46410 | TrGJAroC | BZEMUCCO + h$\nu$ $\rightarrow$ HCOCOHCO3 + C3DIALO2 | jx(ip_HOCH2CHO)*2.+j_ACETOL | Rickard and Pascoe (2009) |
| J46411 | TrGJAroC | BZEMUCCO2H + h$\nu$ $\rightarrow$ C5DIALO2 + $CO_2$ + $HO_2$ | jx(ip_MACR) | Rickard and Pascoe (2009) |
| J46412 | TrGJAroCN | NNCATECOOH + h$\nu$ $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46413 | TrGJAroC | C615CO2OOH + h$\nu$ $\rightarrow$ C5DICARB + CO + $HO_2$ + OH | jx(ip_MVK)+jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46414 | TrGJAroCN | NPHENOOH + h$\nu$ $\rightarrow$ MALDALCO2H + GLYOX + OH + $NO_2$ | j_IC3H7NO3 + jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46415 | TrGJAroCN | NCATECOOH + h$\nu$ $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46416 | TrGJAroC | PBZQOOH + h$\nu$ $\rightarrow$ C5CO2OHCO3 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46417 | TrGJAroC | BZOBIPEROH + h$\nu$ $\rightarrow$ MALDIALCO3 + GLYOX + $HO_2$ | j_ACETOL | Rickard and Pascoe (2009) |
| J46418 | TrGJAroC | BZBIPEROOH + h$\nu$ $\rightarrow$ GLYOX + $HO_2$ + .5 BZFUONE + .5 BZFUONE + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46419 | TrGJAroCN | NBZQOOH + h$\nu$ $\rightarrow$ C6CO4DB + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46420 | TrGJAroC | CATEC1OOH + h$\nu$ $\rightarrow$ CATEC1O + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46421 | TrGJAroC | C6125CO + h$\nu$ $\rightarrow$ C5CO14O2 + CO + $HO_2$ | jx(ip_MGLYOX)+jx(ip_MVK) | Rickard and Pascoe (2009) |
| J46422 | TrGJAroCN | DNPHENOOH + h$\nu$ $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J46423 | TrGJAroC | BZEMUCCO3H + h$\nu$ $\rightarrow$ C5DIALO2 + $CO_2$ + OH | jx(ip_CH3OOH)+jx(ip_MACR) | Rickard and Pascoe (2009) |
| J46424 | TrGJAroC | C6H5OOH + h$\nu$ $\rightarrow$ C6H5O + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J46425 | TrGJAroC | BZEMUCOOH + h$\nu$ $\rightarrow$ .5 EPXC4DIAL + .5 GLYOX + .5 $HO_2$ + .5 C3DIALO2 + .5 C32OH13CO + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009)* |
| J46427 | TrGJAroCN | BZEMUCNO3 + h$\nu$ $\rightarrow$ EPXC4DIAL + $NO_2$ + GLYOX + $HO_2$ | 2.77*jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J46428 | TrGJAroCN | DNPHEN + h$\nu$ $\rightarrow$ HONO + NCPDKETENE | jx(ip_HOC6H4NO2) | Sander et al. (2019) |
| J46429 | TrGJAroCN | NCPDKETENE + h$\nu$ $\rightarrow$ $CO_2$ + CO + 2 $HO_2$ + NC4DCO2H | j_ketene | see note* |
| J47200 | TrGJTerC | CO235C6CHO + h$\nu$ $\rightarrow$ CHOC3COCO3 + $CH_3C(O)$ | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J47201 | TrGJTerC | C235C6CO3H + h$\nu$ $\rightarrow$ CO235C6O2 + $CO_2$ + OH | jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J47202 | TrGJTerC | C716OOH + h$\nu$ $\rightarrow$ CO13C4CHO + $CH_3C(O)$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J47203 | TrGJTerC | C721OOH + h$\nu$ $\rightarrow$ C722O2 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J47204 | TrGJTerC | C722OOH + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + C44O2 + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J47400 | TrGJAroC | TLEPOXMUC + h$\nu$ $\rightarrow$ .5 C615CO2O2 + $HO_2$ + CO + .5 EPXC4DIAL + .5 $CH_3C(O)$ | `4.E3*jx(ip_MVK)*0.1` | Rickard and Pascoe (2009) |
| J47401 | TrGJAroC | C6H5CH2OOH + h$\nu$ $\rightarrow$ BENZAL + $HO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009)* |
| J47402 | TrGJAroCN | C6H5CH2NO3 + h$\nu$ $\rightarrow$ BENZAL + $HO_2$ + $NO_2$ | `0.59*j_IC3H7NO3` | Rickard and Pascoe (2009)* |
| J47403 | TrGJAroC | BENZAL + h$\nu$ $\rightarrow$ $HO_2$ + CO + C6H5O2 | `jx(ip_BENZAL)` | Wallington et al. (2018) |
| J47404 | TrGJAroC | TLBIPEROOH + h$\nu$ $\rightarrow$ .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009)* |
| J47405 | TrGJAroCN | TLBIPERNO3 + h$\nu$ $\rightarrow$ .6 GLYOX + .4 MGLYOX + $HO_2$ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + $NO_2$ | `j_IC3H7NO3` | Rickard and Pascoe (2009)* |
| J47406 | TrGJAroC | TLOBIPEROH + h$\nu$ $\rightarrow$ C5CO14O2 + GLYOX + $HO_2$ | `j_ACETOL` | Rickard and Pascoe (2009) |
| J47407 | TrGJAroC | CRESOOH + h$\nu$ $\rightarrow$ .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009)* |
| J47408a | TrGJAroCN | NCRESOOH + h$\nu$ $\rightarrow$ .68 C5CO14OH + .68 GLYOX + $HO_2$ + .32 PTLQONE + OH + $NO_2$ | `j_IC3H7NO3` | Rickard and Pascoe (2009)* |
| J47408b | TrGJAroCN | NCRESOOH + h$\nu$ $\rightarrow$ C5CO14OH + GLYOX + $NO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009)* |
| J47409 | TrGJAroCN | TOL1OHNO2 + h$\nu$ $\rightarrow$ HONO + MCPDKETENE | `jx(ip_HOPh3Me2NO2)` | see note* |
| J47410 | TrGJAroC | TLEMUCCO2H + h$\nu$ $\rightarrow$ C615CO2O2 + $CO_2$ + $HO_2$ | `jx(ip_MACR)` | Rickard and Pascoe (2009) |
| J47411 | TrGJAroC | TLEMUCCO3H + h$\nu$ $\rightarrow$ C615CO2O2 + $CO_2$ + OH | `jx(ip_CH3OOH)+jx(ip_MACR)` | Rickard and Pascoe (2009) |
| J47412 | TrGJAroC | TLEMUCOOH + h$\nu$ $\rightarrow$ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 $HO_2$ + OH | `jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)+j_ACETOL` | Rickard and Pascoe (2009)* |
| J47413 | TrGJAroCN | TLEMUCNO3 + h$\nu$ $\rightarrow$ EPXC4DIAL + $NO_2$ + $CH_3C(O)$ + CO + $HO_2$ | `2.77*jx(ip_HOCH2CHO)+j_ACETOL` | Rickard and Pascoe (2009) |
| J47414 | TrGJAroC | TLEMUCCO + h$\nu$ $\rightarrow$ $CH_3C(O)$ + EPXC4DIAL + CO + $HO_2$ | `2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)` | Rickard and Pascoe (2009) |
| J47415 | TrGJAroC | C6H5CO3H + h$\nu$ $\rightarrow$ C6H5O2 + $CO_2$ + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J47416 | TrGJAroC | OXYL1OOH + h$\nu$ $\rightarrow$ TOL1O + OH | `jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| J47417 | TrGJAroCN | MNCATECH + h$\nu$ $\rightarrow$ HONO + MCPDKETENE | `jx(ip_HOPh3Me2NO2)` | see note* |
| J47418 | TrGJAroC | MCPDKETENE + h$\nu$ $\rightarrow$ $CO_2$ + CO + 2 $HO_2$ + C4MDIAL | `j_ketene` | see note* |
| J47419 | TrGJAroCN | DNCRES + h$\nu$ $\rightarrow$ HONO + MNCPDKETENE | `jx(ip_HOPh3Me2NO2)` | see note* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J47420 | TrGJAroCN | MNCPDKETENE + h$\nu$ $\rightarrow$ $CO_2$ + CO + 2 $HO_2$ + NC4MDCO2HN | j_ketene | see note* |
| J47421 | TrGJAroC | MCATEC1OOH + h$\nu$ $\rightarrow$ MCATEC1O + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J47422 | TrGJAroCN | NPTLQOOH + h$\nu$ $\rightarrow$ C7CO4DB + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47423 | TrGJAroC | PTLQOOH + h$\nu$ $\rightarrow$ C6CO2OHCO3 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47424 | TrGJAroCN | NCRES1OOH + h$\nu$ $\rightarrow$ NCRES1O + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J47425 | TrGJAroCN | MNNCATCOOH + h$\nu$ $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47426 | TrGJAroCN | MNCATECOOH + h$\nu$ $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47427 | TrGJAroC | C7CO4DB + h$\nu$ $\rightarrow$ C5CO2DBCO3 + $HO_2$ + CO | jx(ip_MGLYOX)*2. | Rickard and Pascoe (2009) |
| J47428 | TrGJAroCN | NDNCRESOOH + h$\nu$ $\rightarrow$ NC4MDCO2HN + $HNO_3$ + CO + CO + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47429 | TrGJAroCN | DNCRESOOH + h$\nu$ $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J47430 | TrGJAroC | C6COOHCO3H + h$\nu$ $\rightarrow$ C5134CO2OH + $HO_2$ + CO + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J48200 | TrGJTerC | C86OOH + h$\nu$ $\rightarrow$ C511O2 + $CH_3COCH_3$ + OH | jx(ip_CH3OOH)+ jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48201 | TrGJTerC | C812OOH + h$\nu$ $\rightarrow$ C813O2 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J48202 | TrGJTerC | C813OOH + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + C512O2 + OH | jx(ip_CH3OOH)+jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J48203 | TrGJTerC | C721CHO + h$\nu$ $\rightarrow$ C721O2 + CO + $HO_2$ | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48204 | TrGJTerC | C721CO3H + h$\nu$ $\rightarrow$ C721O2 + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J48205 | TrGJTerC | C8BCOOH + h$\nu$ $\rightarrow$ C89O2 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J48206 | TrGJTerC | C89OOH + h$\nu$ $\rightarrow$ C810O2 + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48207 | TrGJTerCN | C89NO3 + h$\nu$ $\rightarrow$ C810O2 + $NO_2$ | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48208 | TrGJTerC | C810OOH + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + C514O2 + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48209 | TrGJTerCN | C810NO3 + h$\nu$ $\rightarrow$ $CH_3COCH_3$ + C514O2 + $NO_2$ | 2.84*j_IC3H7NO3+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48210 | TrGJTerCN | C8BCNO3 + h$\nu$ $\rightarrow$ C89O2 + $NO_2$ | j_IC3H7NO3 | Rickard and Pascoe (2009) |
| J48211 | TrGJTerC | C85OOH + h$\nu$ $\rightarrow$ C86O2 + OH | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |
| J48400 | TrGJAroC | STYRENOOH + h$\nu$ $\rightarrow$ $HO_2$ + HCHO + BENZAL + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009)* |
| J49200 | TrGJTerC | C96OOH + h$\nu$ $\rightarrow$ C97O2 + OH | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |
| J49201 | TrGJTerC | C97OOH + h$\nu$ $\rightarrow$ C98O2 + OH | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J49202 | TrGJTerC | C98OOH + h$\nu$ → C614O2 + $CH_3COCH_3$ + OH | (jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)) | Rickard and Pascoe (2009) |
| J49203a | TrGJTerC | NORPINAL + h$\nu$ → C85O2 + CO + $HO_2$ | jx(ip_PINAL2HCO) | Rickard and Pascoe (2009), Sander et al. (2019) |
| J49203b | TrGJTerC | NORPINAL + h$\nu$ → NORPINENOL | jx(ip_PINAL2ENOL) | Sander et al. (2019), Andrews et al. (2012) |
| J49204 | TrGJTerC | C85CO3H + h$\nu$ → C85O2 + $CO_2$ + OH | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |
| J49205 | TrGJTerC | C89CO2H + h$\nu$ → .8 C811CO3 + .2 C89O2 + .2 $CO_2$ + $HO_2$ | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J49206 | TrGJTerC | C89CO3H + h$\nu$ → .8 C811CO3 + .2 C89O2 + .2 $CO_2$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J49207 | TrGJTerC | C811CO3H + h$\nu$ → C811O2 + $CO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J49208 | TrGJTerC | NOPINDOOH + h$\nu$ → C89CO3 + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J40200 | TrGJTerC | LAPINABOOH + h$\nu$ → PINAL + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J40201 | TrGJTerC | MENTHEN6ONE + h$\nu$ → RO6R1O2 + OH | jx(ip_CH3OOH) | Vereecken et al. (2007) |
| J40202 | TrGJTerC | 2OHMENTHEN6ONE + h$\nu$ → 10 LCARBON + OH | jx(ip_CH3OOH) | Vereecken et al. (2007) |
| J40203a | TrGJTerC | PINAL + h$\nu$ → C96O2 + CO + $HO_2$ | jx(ip_PINAL2HCO) | Rickard and Pascoe (2009) |
| J40203b | TrGJTerC | PINAL + h$\nu$ → PINEOL | jx(ip_PINAL2ENOL) | Sander et al. (2019), Andrews et al. (2012)* |
| J40204 | TrGJTerC | PERPINONIC + h$\nu$ → C96O2 + $CO_2$ + OH | jx(ip_CH3OOH)+j_ACETOL | Rickard and Pascoe (2009) |
| J40205 | TrGJTerC | PINALOOH + h$\nu$ → C106O2 + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40206 | TrGJTerCN | PINALNO3 + h$\nu$ → C106O2 + $NO_2$ | j_IC3H7NO3+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40207 | TrGJTerC | C106OOH + h$\nu$ → C716O2 + $CH_3COCH_3$ + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40208 | TrGJTerCN | C106NO3 + h$\nu$ → C716O2 + $CH_3COCH_3$ + $NO_2$ | j_IC3H7NO3+ jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40209 | TrGJTerC | C109OOH + h$\nu$ → C89CO3 + HCHO + OH | jx(ip_CH3OOH)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40210 | TrGJTerC | C109CO + h$\nu$ → C89CO3 + CO + $HO_2$ | jx(ip_MGLYOX)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J40211 | TrGJTerCN | LNAPINABOOH + h$\nu$ → PINAL + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J40212 | TrGJTerC | BPINAOOH + h$\nu$ → NOPINONE + HCHO + $HO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J40213 | TrGJTerCN | LNBPINABOOH + h$\nu$ → NOPINONE + HCHO + $NO_2$ + OH | jx(ip_CH3OOH) | Rickard and Pascoe (2009) |
| J40214 | TrGJTerCN | ROO6R1NO3 + h$\nu$ → ROO6R3O2 + $CH_3COCH_3$ + $NO_2$ | 2.84*j_IC3H7NO3+jx(ip_CH3OOH) | Sander et al. (2019) |
| J40215 | TrGJTerCN | RO6R1NO3 + h$\nu$ → 9 LCARBON + HCHO + $HO_2$ + $NO_2$ | 2.84*j_IC3H7NO3 | Sander et al. (2019) |
| J6000 | StTrGJCl | $Cl_2$ + h$\nu$ → Cl + Cl | jx(ip_Cl2) | Sander et al. (2014) |
| J6100 | StTrGJCl | $Cl_2O_2$ + h$\nu$ → 2 Cl | jx(ip_Cl2O2) | Sander et al. (2014) |
| J6101 | StTrGJCl | OClO + h$\nu$ → ClO + O($^3$P) | jx(ip_OClO) | Sander et al. (2014) |
| J6200 | StGJCl | HCl + h$\nu$ → Cl + H | jx(ip_HCl) | Sander et al. (2014) |
| J6201 | StTrGJCl | HOCl + h$\nu$ → OH + Cl | jx(ip_HOCl) | Sander et al. (2014) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| J6300 | TrGJClN | $ClNO_2 + h\nu \rightarrow Cl + NO_2$ | jx(ip_ClNO2) | Sander et al. (2014) |
| J6301a | StTrGJClN | $ClNO_3 + h\nu \rightarrow Cl + NO_3$ | jx(ip_ClNO3) | Sander et al. (2014) |
| J6301b | StTrGJClN | $ClNO_3 + h\nu \rightarrow ClO + NO_2$ | jx(ip_ClONO2) | Sander et al. (2014) |
| J6400 | StGJCl | $CH_3Cl + h\nu \rightarrow Cl + CH_3$ | jx(ip_CH3Cl) | Sander et al. (2014) |
| J6401 | StGJCl | $CCl_4 + h\nu \rightarrow$ LCARBON + 4 Cl | jx(ip_CCl4) | Sander et al. (2014) |
| J6402 | StGJCCl | $CH_3CCl_3 + h\nu \rightarrow$ 2 LCARBON + 3 Cl | jx(ip_CH3CCl3) | Sander et al. (2014) |
| J6500 | StGJClF | $CFCl_3 + h\nu \rightarrow$ LCARBON + LFLUORINE + 3 Cl | jx(ip_CFCl3) | Sander et al. (2014)* |
| J6501 | StGJClF | $CF_2Cl_2 + h\nu \rightarrow$ LCARBON + 2 LFLUORINE + 2 Cl | jx(ip_CF2Cl2) | Sander et al. (2014)* |
| J7000 | StTrGJBr | $Br_2 + h\nu \rightarrow Br + Br$ | jx(ip_Br2) | Sander et al. (2014) |
| J7100 | StTrGJBr | $BrO + h\nu \rightarrow Br + O(^3P)$ | jx(ip_BrO) | Sander et al. (2014) |
| J7200 | StTrGJBr | $HOBr + h\nu \rightarrow Br + OH$ | jx(ip_HOBr) | Sander et al. (2014) |
| J7300 | TrGJBrN | $BrNO_2 + h\nu \rightarrow Br + NO_2$ | jx(ip_BrNO2) | Sander et al. (2014) |
| J7301 | StTrGJBrN | $BrNO_3 + h\nu \rightarrow .85\ Br + .85\ NO_3 + .15\ BrO + .15\ NO_2$ | jx(ip_BrNO3) | Sander et al. (2014)* |
| J7400 | StGJBr | $CH_3Br + h\nu \rightarrow Br + CH_3$ | jx(ip_CH3Br) | Sander et al. (2014) |
| J7401 | TrGJBr | $CH_2Br_2 + h\nu \rightarrow$ LCARBON + 2 Br | jx(ip_CH2Br2) | Sander et al. (2014) |
| J7402 | TrGJBr | $CHBr_3 + h\nu \rightarrow$ LCARBON + 3 Br | jx(ip_CHBr3) | Sander et al. (2014) |
| J7500 | StGJBrF | $CF_3Br + h\nu \rightarrow$ LCARBON + 3 LFLUORINE + Br | jx(ip_CF3Br) | Sander et al. (2014) |
| J7600 | StTrGJBrCl | $BrCl + h\nu \rightarrow Br + Cl$ | jx(ip_BrCl) | Sander et al. (2014) |
| J7601 | StGJBrClF | $CF_2ClBr + h\nu \rightarrow$ LCARBON + 2 LFLUORINE + Br + Cl | jx(ip_CF2ClBr) | Sander et al. (2014) |
| J7602 | TrGJBrCl | $CH_2ClBr + h\nu \rightarrow$ LCARBON + Br + Cl | jx(ip_CH2ClBr) | Sander et al. (2014) |
| J7603 | TrGJBrCl | $CHCl_2Br + h\nu \rightarrow$ LCARBON + Br + 2 Cl | jx(ip_CHCl2Br) | Sander et al. (2014) |
| J7604 | TrGJBrCl | $CHClBr_2 + h\nu \rightarrow$ LCARBON + 2 Br + Cl | jx(ip_CHClBr2) | Sander et al. (2014) |
| J8000 | TrGJI | $I_2 + h\nu \rightarrow I + I$ | jx(ip_I2) | Sander et al. (2014) |
| J8100 | TrGJI | $IO + h\nu \rightarrow I + O(^3P)$ | jx(ip_IO) | Sander et al. (2014) |
| J8200 | TrGJI | $HOI + h\nu \rightarrow I + OH$ | jx(ip_HOI) | Sander et al. (2014) |
| J8300 | TrGJIN | $INO_2 + h\nu \rightarrow I + NO_2$ | jx(ip_INO2) | Sander et al. (2014) |
| J8301 | TrGJIN | $INO_3 + h\nu \rightarrow I + NO_3$ | jx(ip_INO3) | Sander et al. (2014) |
| J8400 | TrGJI | $CH_2I_2 + h\nu \rightarrow 2\ I + 2\ HO_2 + CO$ | jx(ip_CH2I2) | Sander et al. (2014) |
| J8401 | TrGJI | $CH_3I + h\nu \rightarrow I + CH_3$ | jx(ip_CH3I) | Sander et al. (2014) |
| J8402 | TrGJCI | $CH_3CHICH_3 + h\nu \rightarrow$ 2 LCARBON + I + $CH_3$ | jx(ip_C3H7I) | Sander et al. (2014) |
| J8403 | TrGJClI | $CH_2ClI + h\nu \rightarrow I + Cl + 2\ HO_2 + CO$ | jx(ip_CH2ClI) | Sander et al. (2014) |
| J8600 | TrGJClI | $ICl + h\nu \rightarrow I + Cl$ | jx(ip_ICl) | Sander et al. (2014) |
| J8700 | TrGJBrI | $IBr + h\nu \rightarrow I + Br$ | jx(ip_IBr) | Sander et al. (2014) |
| PH (aqueous) | | | | |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| PH2100_a01 | TrAa01ScJ | $H_2O_2$(aq) + h$\nu$ $\rightarrow$ 2 OH(aq) | `2.33*xaer(01)*jx(ip_H2O2)` | see note* |
| PH3200_a01 | TrAa01JN | $NO_3^-$(aq) + h$\nu$ $\rightarrow$ $NO_2$(aq) + OH(aq) + $OH^-$(aq) | `xaer(01)*jx(ip_NO2) * 1.4E-4` | see note* |
| PH4100_a01 | TrAa01ScJ | $HOCH_2OOH$(aq) + h$\nu$ $\rightarrow$ HCOOH(aq) + OH(aq) + $HO_2$(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | Sander et al. (2014) |
| PH4101_a01 | TrAa01ScJ | $CH_3OOH$(aq) + h$\nu$ $\rightarrow$ HCHO(aq) + OH(aq) + $HO_2$(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | Sander et al. (2014) |
| PH4200_a01 | TrAa01ScJC | C2H5OOH(aq) + h$\nu$ $\rightarrow$ $CH_3CHO$(aq) + $HO_2$(aq) + OH(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | von Kuhlmann (2001)* |
| PH4201_a01 | TrAa01ScJC | HOOCH2CO2H(aq) + h$\nu$ $\rightarrow$ HCHO(aq) + $CO_2$(aq) + $HO_2$(aq) + OH(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | Rickard and Pascoe (2009)* |
| PH4202_a01 | TrAa01ScJC | $CH_2OOHCO_2^-$(aq) + h$\nu$ $\rightarrow$ $CHOHOOCOO_2^-$(aq) + OH(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | see note* |
| PH4203_a01 | TrAa01ScJC | $CH_3C(O)OOH$(aq) + h$\nu$ $\rightarrow$ $CH_3OO$(aq) + $CO_2$(aq) + OH(aq) | `2.33*xaer(01)*jx(ip_CH3CO3H)` | Sander et al. (2014) |
| PH4204_a01 | TrAa01ScJC | $HOCH_2CO_3H$(aq) + h$\nu$ $\rightarrow$ HCHO(aq) + OH(aq) + $HO_2$(aq) + $CO_2$(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | Rickard and Pascoe (2009) |
| PH4205_a01 | TrAa01ScJC | $CH_3CHO$(aq) + h$\nu$ $\rightarrow$ $CH_3OO$(aq) + $HO_2$(aq) + CO(aq) | `2.33*xaer(01)*jx(ip_CH3CHO)` | Sander et al. (2014) |
| PH4206_a01 | TrAa01ScJC | $CH_2OOHCHO$(aq) + h$\nu$ $\rightarrow$ OH(aq) + HCHO(aq) + CO(aq) + $HO_2$(aq) | `2.33*xaer(01)*(jx(ip_CH3OOH) +jx(ip_HOCH2CHO))` | Sander et al. (2019) |
| PH4207a_a01 | TrAa01ScJC | $CH_2OHCHO$(aq) + h$\nu$ $\rightarrow$ HCHO(aq) + 2 $HO_2$(aq) + CO(aq) | `2.33*xaer(01)*jx(ip_HOCH2CHO) *0.83` | Sander et al. (2014)* |
| PH4207b_a01 | TrAa01ScJC | $CH_2OHCHO$(aq) + h$\nu$ $\rightarrow$ OH(aq) + .6 HCHO(aq) + .6 CO(aq) + .6 $HO_2$(aq) + .2 GLYOX(aq) + .2 $CH_2OHCHO$(aq) | `2.33*xaer(01)*jx(ip_HOCH2CHO) *0.07` | Sander et al. (2014)* |
| PH4207c_a01 | TrAa01ScJC | $CH_2OHCHO$(aq) + h$\nu$ $\rightarrow$ $CH_3OH$(aq) + CO(aq) | `2.33*xaer(01)*jx(ip_HOCH2CHO) *0.10` | Sander et al. (2014)* |
| PH4208_a01 | TrAa01ScJC | CHOCOOH(aq) + h$\nu$ $\rightarrow$ 2 $HO_2$(aq) + CO(aq) + $CO_2$(aq) | `2.33*xaer(01)*jx(ip_MGLYOX)` | Rickard and Pascoe (2009) |
| PH4209_a01 | TrAa01ScJC | GLYOX(aq) + h$\nu$ $\rightarrow$ 2 CO(aq) + 2 $HO_2$(aq) | `2.33*xaer(01)*jx(ip_GLYOX)` | Sander et al. (2014) |
| PH4210a_a01 | TrAa01ScJC | HOOCCOOH(aq) + h$\nu$ $\rightarrow$ $CO_2$(aq) + HCOOH(aq) | `2.33*xaer(01)*0.72*jx(ip_ HOOCCOOH)` | Yamamoto and Back (1985) |
| PH4210b_a01 | TrAa01ScJC | HOOCCOOH(aq) + h$\nu$ $\rightarrow$ $CO_2$(aq) + CO(aq) + $H_2O$(aq) | `2.33*xaer(01)*0.28*jx(ip_ HOOCCOOH)` | Yamamoto and Back (1985) |
| PH4211_a01 | TrAa01ScJC | CHOCHOHOH(aq) + h$\nu$ $\rightarrow$ HCOOH(aq) + 2 $HO_2$(aq) + CO(aq) | `2.33*xaer(01)*jx(ip_HOCH2CHO)` | Sander et al. (2014)* |
| PH4300_a01 | TrAa01ScJC | $CH_3COCH_2O_2H$(aq) + h$\nu$ $\rightarrow$ $CH_3COOO$(aq) + HCHO(aq) + OH(aq) | `2.33*xaer(01)*(jx(ip_CH3OOH) +0.65*0.11*jx(ip_CHOH))` | see note* |
| PH4301_a01 | TrAa01ScJC | $iC_3H_7OOH$(aq) + h$\nu$ $\rightarrow$ $CH_3COCH_3$(aq) + $HO_2$(aq) + OH(aq) | `2.33*xaer(01)*jx(ip_CH3OOH)` | see note* |
| PH4302_a01 | TrAa01ScJC | $CH_3COCH_2OH$(aq) + h$\nu$ $\rightarrow$ .5 OH(aq) + .5 HCHO(aq) + .5 CO(aq) + .5 HCHO(aq) + .5 $HO_2$(aq) + .5 $CH_2OHCO3$(aq) + .5 $CH_3OO$(aq) | `2.33*xaer(01)*0.65*0.11*jx(ip_ CHOH)` | Sander et al. (2014)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| PH4303_a01 | TrAa01ScJC | $CH_3C(O)CHO(aq) + h\nu \rightarrow OH(aq) + HCHO(aq) + CO(aq) + CO(aq) + HO_2(aq)$ | 2.33*xaer(01)*jx(ip_MGLYOX) | Sander et al. (2014)* |
| PH10200_a01 | TrAa01JHg | $Hg(OH)_2(aq) + h\nu \rightarrow Hg(aq)$ | xaer(01)*6E-5*jx(ip_NO2) | see note* |
| PH11200_a01 | TrAa01JFe | $FeOH^{2+}(aq) + h\nu \rightarrow Fe^{2+}(aq) + OH(aq)$ | xaer(01)*4.51E-3*0.312 | Herrmann et al. (2000) |
| PH11201_a01 | TrAa01JFe | $Fe(OH)_2^+(aq) + h\nu \rightarrow Fe^{2+}(aq) + OH(aq) + OH^-(aq)$ | xaer(01)*5.77E-3*0.255 | Herrmann et al. (2000) |
| PH11800_a01 | TrAa01JFeS | $FeSO_4^+(aq) + h\nu \rightarrow Fe^{2+}(aq) + SO_4^-(aq)$ | xaer(01)*6.43E-3*7.9E-3 | Herrmann et al. (2000) |

# General notes

*j*-values are calculated with an external module (e.g., JVAL) and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:
j(11) → jx(ip_COH2)
j(12) → jx(ip_CHOH)
j(15) → jx(ip_HOCH2CHO)
j(18) → jx(ip_MACR)
j(22) → jx(ip_ACETOL)
j(23)+j(24) → jx(ip_MVK)
j(31)+j(32)+j(33) → jx(ip_GLYOX)
j(34) → jx(ip_MGLYOX)
j(41) → jx(ip_CH3OOH)
j(53) → j(isopropyl nitrate)
j(54) → j(isopropyl nitrate)
j(55) → j(isopropyl nitrate)
j(56)+j(57) → jx(ip_NOA)

# Specific notes

J41003: $CH_3$- and $CH_2$-channels are considered only and with their branching ratios being 0.42 and 0.48, respectively (Gans et al., 2011). CH-production is neglected. $CH_2$ is assumed to react only with O2 yielding 1.44 $H_2$ + 0.18 HCHO + 0.18 $O(^3P)$ + 0.33 OH + 0.33 $HO_2$ + 0.44 $CO_2$ + 0.38 CO + 0.05 $H_2O$ as assumed in the WACCM model by J. Orlando (Doug Kinnison, pers. comm. with D. Taraborrelli).

J41006: product distribution as for HNO4

J42004: Quantum yields from Burkholder et al. (2015).

J42005a: Quantum yields from Burkholder et al. (2015).

J42005b: Quantum yields from Burkholder et al. (2015).

J42005c: Quantum yields from Burkholder et al. (2015).

J42007: It is assumed that J(PHAN) is the same as J(PAN).

J42017: Enhancement of j according to Müller et al. (2014).

J42020: It is assumed that j($NO_3$CH2CHO) is the same as j(PAN).

J42021: In analogy to what is assumed for $CH_3O_2NO_2$ photolysis as in (Sander et al., 2014).

J43002: Following von Kuhlmann et al. (2003), we use j($CH_3COCH_2OH$) = 0.11*jx(ip_CHOH). As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a).

J43006: Following von Kuhlmann et al. (2003), we use J($iC_3H_7ONO_2$) = 3.7*jx(ip_PAN).

J43018: One third of the acetaldehyde channel is considered to be CH2CHOH according to Hjorth (2002) EUPHORE Report.

J43024: Assuming J($C_3H_7ONO_2$) = 0.59 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J43025a: Photolysis frequencies very similar to the ones of $CH_3CHO$.

J43025b: Photolysis frequencies very similar to the ones of $CH_3CHO$.

J43400: KDEC C3DIALO → GLYOX + CO + HO2

J44004: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44005a: It is assumed that J(LC4H9NO3) is the same as J($iC_3H_7ONO_2$).

J44005b: It is assumed that J(LC4H9NO3) is the same as J($iC_3H_7ONO_2$).

J44006: It is assumed that J(MPAN) is the same as J(PAN).

J44009: It is assumed that J(MACROOH) is 2.77 times larger than J($HOCH_2CHO$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44010: It is assumed that J(MACROH) is 2.77 times larger than J($HOCH_2CHO$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44015: It is assumed that J(BIACETOH) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44017a: CO-channel yielding $CH_3COCH$ which upon reaction with $O_2$ produces an excited Criegee Intermediate assumed to be similar to MGLOOA in MCM. MGLOOA is produced also in other reactions and is substituted by its decomposition products. Furthermore, the stabilized Criegge Intermediate is assumed to solely react with water.

J44025: J values only for the secondary nitrate.

J44026: Like for LMEKNO3 photolysis

J44027: 2.84*J_IC3H7NO3 like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to Müller et al. (2014).

J44037b: Channel which produces just vinyl alcohol and not a larger enol via keto-enol phototautomerization.

J44043: The resulting vinyl peroxy radical is assumed to mostly form with $HO_2$ a labile hydroperoxide (see ketene formation). The products are further simplified.

J44044: 1,5-H-shift for the resulting vinyl peroxy radical assumed to be dominant.

J44046a: Simplified oxidation.

J44400b: KDEC MALDIALO → GLYOX + GLYOX + HO2

J44401: KDEC BZFUO → CO14O3CHO + HO2

J44403: KDEC NBZFUO → 0.5 CO14O3CHO + 0.5 NO2 + 0.5 NBZFUONE + 0.5 HO2

J44404b: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO

J44407: KDEC MALANHYO → HCOCOHCO3

J44414: KDEC MECOACETO → CH3CO3 + HCHO

J45003: It is assumed that J(LISOPACNO3) = 0.59 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that J(ISOPBNO3) = 2.84 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that J(ISOPDNO3) is the same as J($iC_3H_7ONO_2$).

J45009: 0.59*J_IC3H7NO3 like for other primary alkyl nitrates (see J4503). Enhancement of J according to Müller et al. (2014).

J45015: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that J(HCOC5) is half as large as J(MVK). With exeption of HOCH2CO the products of MACO2 decomposition without $CO_2$.

J45032: approximation with 4-oxo-pentenal photolysis combining results of Thner et al(2004) and Xiang et al(2007)

J45402: KDEC C5DIALO → MALDIAL + CO + HO2

J45407: KDEC TLFUONE → 0.6 C5CO14O2 + 0.6 HO2 + 0.4 TLFUONE

J45410: KDEC MMALANHYO → CO2H3CO3

J45411: KDEC C5DICARBO → MGLYOX + GLYOX + HO2

J45412: KDEC NTLFUO → ACCOMECHO + NO2

J45414: KDEC C5CO14CO2 → 0.83 MALANHY + 0.83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

J45415: KDEC TLFUO → ACCOMECHO + HO2

J46400: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

J46403: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

J46404: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

J46415: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

J46416: KDEC PBZQO → C5CO2OHCO3

J46418: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

J46419: KDEC NBZQO → C6CO4DB + NO2

J46422: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

J46425: KDEC BZEMUCO → 0.5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

J46429: new channel

J47401: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2

J47402: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2

J47404: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 C4MDIAL + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47405: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 C4MDIAL + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47407: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

J47408a: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

J47408b: KDEC NCRESO → C5CO14OH + GLYOX + NO2

J47409: Using J for 3-methyl-2-nitrophenol.

J47412: KDEC TLEMUCO → 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

J47417: Using J for 3-methyl-2-nitrophenol.

J47418: new channel

J47419: Using J for 3-methyl-2-nitrophenol.

J47420: new channel

J47422: KDEC NPTLQO → C7CO4DB + NO2

J47423: KDEC PTLQO → C6CO2OHCO3

J47425: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

J47426: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

J47428: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

J47429: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

J48400: KDEC STYRENO → HO2 + HCHO + BENZAL

J40203b: Substituted vinyl alcohol in analogy to $CH_3CHO$ photolysis.

J6500: Even though the elementary reaction produces only 1 Cl atom (Felder and Demuth, 1993), it is assumed here that eventually all Cl atoms are released in secondary reactions.

J6501: Even though the elementary reaction probably produces only 1 Cl atom (as for $CFCl_3$), it is assumed here that eventually all Cl atoms are released in secondary reactions.

J7301: The quantum yields are recommended by Burkholder et al. (2015) for $\lambda > 300$nm and used here for the entire spectrum.

PH2100_a01: 2.33 times the gas-phase value

PH3200_a01: Scaled to $J(NO_2)$ so that its lifetime is about 10.5 days, as suggested by Zellner et al. (1990).

PH4200_a01: CH3CHOHO2 is assumed to directly decompose into CH3CHO + HO2

PH4201_a01: COOHOO is not formed but directly dissociates into CO2 + HO2

PH4202_a01: assumed to be the same as C2H5OOH + hv

PH4207a_a01: Quantum yields from Burkholder et al. (2015).

PH4207b_a01: Quantum yields from Burkholder et al. (2015). HCOCH2O2 decomposes directly to .6 HCHO + .6 CO + .6 HO2 + .2 GLYOX + .2 HOCH2CHO

PH4207c_a01: Quantum yields from Burkholder et al. (2015).

PH4211_a01: Assumed in analogy to the main channel for $j$(HOCH2CHO).

PH4300_a01: 2.33* $k$ from the gas-phase reaction, CH3CO directly reacts with O2 to form CH3CO3

PH4301_a01: 2.33 * $k$ from the gas-phase reaction,

PH4302_a01: Following von Kuhlmann et al. (2003), we use $j(CH_3COCH_2OH)$ = `0.11*jx(ip_CHOH)`. As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a). CH3CO reacts with O2 to form OH + HCHO + CO. HOCH2CO reacts with O2 to form HOCH2CO3

PH4303_a01: CH3CO reacts with O2 to form OH + HCHO + CO

PH10200_a01: Scaled to $J(NO_2)$ so that it produces about $3.0 \times 10^{-7}$.

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H10000f_a01 | TrAa01Sc | $O_2 \rightarrow O_2(aq)$ | k_exf(01,ind_O2) | see general notes* |
| H10000b_a01 | TrAa01Sc | $O_2(aq) \rightarrow O_2$ | k_exb(01,ind_O2) | see general notes* |
| H10001f_a01 | TrAa01MblScScm | $O_3 \rightarrow O_3(aq)$ | k_exf(01,ind_O3) | see general notes* |
| H10001b_a01 | TrAa01MblScScm | $O_3(aq) \rightarrow O_3$ | k_exb(01,ind_O3) | see general notes* |
| H21000f_a01 | TrAa01Sc | $OH \rightarrow OH(aq)$ | k_exf(01,ind_OH) | see general notes* |
| H21000b_a01 | TrAa01Sc | $OH(aq) \rightarrow OH$ | k_exb(01,ind_OH) | see general notes* |
| H21001f_a01 | TrAa01Sc | $HO_2 \rightarrow HO_2(aq)$ | k_exf(01,ind_HO2) | see general notes* |
| H21001b_a01 | TrAa01Sc | $HO_2(aq) \rightarrow HO_2$ | k_exb(01,ind_HO2) | see general notes* |
| H21002f_a01 | TrAa01MblScScm | $H_2O_2 \rightarrow H_2O_2(aq)$ | k_exf(01,ind_H2O2) | see general notes* |
| H21002b_a01 | TrAa01MblScScm | $H_2O_2(aq) \rightarrow H_2O_2$ | k_exb(01,ind_H2O2) | see general notes* |
| H31000f_a01 | TrAa01ScN | $NO \rightarrow NO(aq)$ | k_exf(01,ind_NO) | see general notes* |
| H31000b_a01 | TrAa01ScN | $NO(aq) \rightarrow NO$ | k_exb(01,ind_NO) | see general notes* |
| H31001f_a01 | TrAa01ScN | $NO_2 \rightarrow NO_2(aq)$ | k_exf(01,ind_NO2) | see general notes* |
| H31001b_a01 | TrAa01ScN | $NO_2(aq) \rightarrow NO_2$ | k_exb(01,ind_NO2) | see general notes* |
| H31002f_a01 | TrAa01ScN | $NO_3 \rightarrow NO_3(aq)$ | k_exf(01,ind_NO3) | see general notes* |
| H31002b_a01 | TrAa01ScN | $NO_3(aq) \rightarrow NO_3$ | k_exb(01,ind_NO3) | see general notes* |
| H32000f_a01 | TrAa01MblScScmN | $NH_3 \rightarrow NH_3(aq)$ | k_exf(01,ind_NH3) | see general notes* |
| H32000b_a01 | TrAa01MblScScmN | $NH_3(aq) \rightarrow NH_3$ | k_exb(01,ind_NH3) | see general notes* |
| H32001_a01 | TrAa01MblScScmN | $N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$ | k_exf_N2O5(01)*C(ind_H2O_a01) | Behnke et al. (1994), Behnke et al. (1997) |
| H32002f_a01 | TrAa01ScN | $HONO \rightarrow HONO(aq)$ | k_exf(01,ind_HONO) | see general notes* |
| H32002b_a01 | TrAa01ScN | $HONO(aq) \rightarrow HONO$ | k_exb(01,ind_HONO) | see general notes* |
| H32003f_a01 | TrAa01MblScScmN | $HNO_3 \rightarrow HNO_3(aq)$ | k_exf(01,ind_HNO3) | see general notes* |
| H32003b_a01 | TrAa01MblScScmN | $HNO_3(aq) \rightarrow HNO_3$ | k_exb(01,ind_HNO3) | see general notes* |
| H32004f_a01 | TrAa01ScN | $HNO_4 \rightarrow HNO_4(aq)$ | k_exf(01,ind_HNO4) | see general notes* |
| H32004b_a01 | TrAa01ScN | $HNO_4(aq) \rightarrow HNO_4$ | k_exb(01,ind_HNO4) | see general notes* |
| H41000f_a01 | TrAa01MblScScm | $CO_2 \rightarrow CO_2(aq)$ | k_exf(01,ind_CO2) | see general notes* |
| H41000b_a01 | TrAa01MblScScm | $CO_2(aq) \rightarrow CO_2$ | k_exb(01,ind_CO2) | see general notes* |
| H41001f_a01 | TrAa01ScScm | $HCHO \rightarrow HCHO(aq)$ | k_exf(01,ind_HCHO) | see general notes* |
| H41001b_a01 | TrAa01ScScm | $HCHO(aq) \rightarrow HCHO$ | k_exb(01,ind_HCHO) | see general notes* |
| H41002f_a01 | TrAa01Sc | $CH_3O_2 \rightarrow CH_3OO(aq)$ | k_exf(01,ind_CH3O2) | see general notes* |
| H41002b_a01 | TrAa01Sc | $CH_3OO(aq) \rightarrow CH_3O_2$ | k_exb(01,ind_CH3O2) | see general notes* |
| H41003f_a01 | TrAa01ScScm | $HCOOH \rightarrow HCOOH(aq)$ | k_exf(01,ind_HCOOH) | see general notes* |
| H41003b_a01 | TrAa01ScScm | $HCOOH(aq) \rightarrow HCOOH$ | k_exb(01,ind_HCOOH) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H41004f_a01 | TrAa01ScScm | $CH_3OOH \rightarrow CH_3OOH(aq)$ | k_exf(01,ind_CH3OOH) | see general notes* |
| H41004b_a01 | TrAa01ScScm | $CH_3OOH(aq) \rightarrow CH_3OOH$ | k_exb(01,ind_CH3OOH) | see general notes* |
| H41005f_a01 | TrAa01Sc | $CH_3OH \rightarrow CH_3OH(aq)$ | k_exf(01,ind_CH3OH) | see general notes* |
| H41005b_a01 | TrAa01Sc | $CH_3OH(aq) \rightarrow CH_3OH$ | k_exb(01,ind_CH3OH) | see general notes* |
| H41006f_a01 | TrAa01Sc | $HOCH_2OH \rightarrow HOCH_2OH(aq)$ | k_exf(01,ind_HOCH2OH) | see general notes* |
| H41006b_a01 | TrAa01Sc | $HOCH_2OH(aq) \rightarrow HOCH_2OH$ | k_exb(01,ind_HOCH2OH) | see general notes* |
| H41007f_a01 | TrAa01Sc | $HOCH_2OOH \rightarrow HOCH_2OOH(aq)$ | k_exf(01,ind_HOCH2OOH) | see general notes* |
| H41007b_a01 | TrAa01Sc | $HOCH_2OOH(aq) \rightarrow HOCH_2OOH$ | k_exb(01,ind_HOCH2OOH) | see general notes* |
| H41008f_a01 | TrAa01Sc | $CO \rightarrow CO(aq)$ | k_exf(01,ind_CO) | see general notes* |
| H41008b_a01 | TrAa01Sc | $CO(aq) \rightarrow CO$ | k_exb(01,ind_CO) | see general notes* |
| H42000f_a01 | TrAa01ScScmC | $CH_3COOH \rightarrow CH_3COOH(aq)$ | k_exf(01,ind_CH3CO2H) | see general notes* |
| H42000b_a01 | TrAa01ScScmC | $CH_3COOH(aq) \rightarrow CH_3COOH$ | k_exb(01,ind_CH3CO2H) | see general notes* |
| H42001f_a01 | TrAa01ScC | $CH_3CHO \rightarrow CH_3CHO(aq)$ | k_exf(01,ind_CH3CHO) | see general notes* |
| H42001b_a01 | TrAa01ScC | $CH_3CHO(aq) \rightarrow CH_3CHO$ | k_exb(01,ind_CH3CHO) | see general notes* |
| H42002f_a01 | TrAa01ScCN | $PAN \rightarrow PAN(aq)$ | k_exf(01,ind_PAN) | see general notes* |
| H42002b_a01 | TrAa01ScCN | $PAN(aq) \rightarrow PAN$ | k_exb(01,ind_PAN) | see general notes* |
| H42003f_a01 | TrAa01ScC | $C_2H_5OH \rightarrow CH_3CH_2OH(aq)$ | k_exf(01,ind_C2H5OH) | see general notes* |
| H42003b_a01 | TrAa01ScC | $CH_3CH_2OH(aq) \rightarrow C_2H_5OH$ | k_exb(01,ind_C2H5OH) | see general notes* |
| H42004f_a01 | TrAa01ScC | $ETHGLY \rightarrow ETHGLY(aq)$ | k_exf(01,ind_ETHGLY) | see general notes* |
| H42004b_a01 | TrAa01ScC | $ETHGLY(aq) \rightarrow ETHGLY$ | k_exb(01,ind_ETHGLY) | see general notes* |
| H42006f_a01 | TrAa01ScC | $CH_3C(O)OO \rightarrow CH_3COOO(aq)$ | k_exf(01,ind_CH3CO3) | see general notes* |
| H42006b_a01 | TrAa01ScC | $CH_3COOO(aq) \rightarrow CH_3C(O)OO$ | k_exb(01,ind_CH3CO3) | see general notes* |
| H42007f_a01 | TrAa01ScC | $HOCH_2CHO \rightarrow CH_2OHCHO(aq)$ | k_exf(01,ind_HOCH2CHO) | see general notes* |
| H42007b_a01 | TrAa01ScC | $CH_2OHCHO(aq) \rightarrow HOCH_2CHO$ | k_exb(01,ind_HOCH2CHO) | see general notes* |
| H42008f_a01 | TrAa01ScC | $GLYOX \rightarrow GLYOX(aq)$ | k_exf(01,ind_GLYOX) | see general notes* |
| H42008b_a01 | TrAa01ScC | $GLYOX(aq) \rightarrow GLYOX$ | k_exb(01,ind_GLYOX) | see general notes* |
| H42009f_a01 | TrAa01ScC | $CH_3C(O)OOH \rightarrow CH_3C(O)OOH(aq)$ | k_exf(01,ind_CH3CO3H) | see general notes* |
| H42009b_a01 | TrAa01ScC | $CH_3C(O)OOH(aq) \rightarrow CH_3C(O)OOH$ | k_exb(01,ind_CH3CO3H) | see general notes* |
| H42010f_a01 | TrAa01ScC | $HOCH_2CO_3H \rightarrow HOCH_2CO_3H(aq)$ | k_exf(01,ind_HOCH2CO3H) | see general notes* |
| H42010b_a01 | TrAa01ScC | $HOCH_2CO_3H(aq) \rightarrow HOCH_2CO_3H$ | k_exb(01,ind_HOCH2CO3H) | see general notes* |
| H42011f_a01 | TrAa01ScC | $C_2H_5OOH \rightarrow$ C2H5OOH(aq) | k_exf(01,ind_C2H5OOH) | see general notes* |
| H42011b_a01 | TrAa01ScC | C2H5OOH(aq) $\rightarrow C_2H_5OOH$ | k_exb(01,ind_C2H5OOH) | see general notes* |
| H42012f_a01 | TrAa01ScC | $HOOCCOOH \rightarrow HOOCCOOH(aq)$ | k_exf(01,ind_HOOCCOOH) | see general notes* |
| H42012b_a01 | TrAa01ScC | $HOOCCOOH(aq) \rightarrow HOOCCOOH$ | k_exb(01,ind_HOOCCOOH) | see general notes* |
| H42013f_a01 | TrAa01ScC | HOOCH2CO2H $\rightarrow$ HOOCH2CO2H(aq) | k_exf(01,ind_HOOCH2CO2H) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H42013b_a01 | TrAa01ScC | HOOCH2CO2H(aq) $\rightarrow$ HOOCH2CO2H | k_exb(01,ind_HOOCH2CO2H) | see general notes* |
| H42014f_a01 | TrAa01ScC | $HOCH_2CO_2H \rightarrow HOCH_2CO_2H(aq)$ | k_exf(01,ind_HOCH2CO2H) | see general notes* |
| H42014b_a01 | TrAa01ScC | $HOCH_2CO_2H(aq) \rightarrow HOCH_2CO_2H$ | k_exb(01,ind_HOCH2CO2H) | see general notes* |
| H42015f_a01 | TrAa01ScC | $HCOCO_2H \rightarrow CHOCOOH(aq)$ | k_exf(01,ind_HCOCO2H) | see general notes* |
| H42015b_a01 | TrAa01ScC | $CHOCOOH(aq) \rightarrow HCOCO_2H$ | k_exb(01,ind_HCOCO2H) | see general notes* |
| H42017f_a01 | TrAa01ScCN | $C_2H_5ONO_2 \rightarrow C_2H_5ONO_2(aq)$ | k_exf(01,ind_C2H5NO3) | see general notes* |
| H42017b_a01 | TrAa01ScCN | $C_2H_5ONO_2(aq) \rightarrow C_2H_5ONO_2$ | k_exb(01,ind_C2H5NO3) | see general notes* |
| H42018f_a01 | TrAa01ScCN | $CH_3CN \rightarrow CH_3CN(aq)$ | k_exf(01,ind_CH3CN) | see general notes* |
| H42018b_a01 | TrAa01ScCN | $CH_3CN(aq) \rightarrow CH_3CN$ | k_exb(01,ind_CH3CN) | see general notes* |
| H42019f_a01 | TrAa01ScC | $HOCH_2CHOHOH \rightarrow CH_2OHCHOHOH(aq)$ | k_exf(01,ind_HOCH2CHOHOH) | see general notes* |
| H42019b_a01 | TrAa01ScC | $CH_2OHCHOHOH(aq) \rightarrow HOCH_2CHOHOH$ | k_exb(01,ind_HOCH2CHOHOH) | see general notes* |
| H42020f_a01 | TrAa01ScC | $CH_3CHOHOH \rightarrow CH_3CHOHOH(aq)$ | k_exf(01,ind_CH3CHOHOH) | see general notes* |
| H42020b_a01 | TrAa01ScC | $CH_3CHOHOH(aq) \rightarrow CH_3CHOHOH$ | k_exb(01,ind_CH3CHOHOH) | see general notes* |
| H42021f_a01 | TrAa01ScC | CHOHOHCOOH $\rightarrow$ CHOOHOHCOOH(aq) | k_exf(01,ind_CHOHOHCOOH) | see general notes* |
| H42021b_a01 | TrAa01ScC | CHOOHOHCOOH(aq) $\rightarrow$ CHOHOHCOOH | k_exb(01,ind_CHOHOHCOOH) | see general notes* |
| H42022f_a01 | TrAa01ScC | CHOHOHCHOHOH $\rightarrow$ CHOHOHCHOHOH(aq) | k_exf(01,ind_CHOHOHCHOHOH) | see general notes* |
| H42022b_a01 | TrAa01ScC | CHOHOHCHOHOH(aq) $\rightarrow$ CHOHOHCHOHOH | k_exb(01,ind_CHOHOHCHOHOH) | see general notes* |
| H42023f_a01 | TrAa01ScC | HOOCH2CHO $\rightarrow$ $CH_2OOHCHO(aq)$ | k_exf(01,ind_HOOCH2CHO) | see general notes* |
| H42023b_a01 | TrAa01ScC | $CH_2OOHCHO(aq)$ $\rightarrow$ HOOCH2CHO | k_exb(01,ind_HOOCH2CHO) | see general notes* |
| H42024f_a01 | TrAa01ScC | CHOCHOHOH $\rightarrow$ CHOCHOHOH(aq) | k_exf(01,ind_CHOCHOHOH) | see general notes* |
| H42024b_a01 | TrAa01ScC | CHOCHOHOH(aq) $\rightarrow$ CHOCHOHOH | k_exb(01,ind_CHOCHOHOH) | see general notes* |
| H42025f_a01 | TrAa01ScC | $HOOCH_2CHOHOH \rightarrow HOOCH_2CHOHOH(aq)$ | k_exf(01,ind_HOOCH2CHOHOH) | see general notes* |
| H42025b_a01 | TrAa01ScC | $HOOCH_2CHOHOH(aq) \rightarrow HOOCH_2CHOHOH$ | k_exb(01,ind_HOOCH2CHOHOH) | see general notes* |
| H42026f_a01 | TrAa01ScC | CH2CO $\rightarrow$ CH2CO(aq) | k_exf(01,ind_CH2CO) | see general notes* |
| H42026b_a01 | TrAa01ScC | CH2CO(aq) $\rightarrow$ CH2CO | k_exb(01,ind_CH2CO) | see general notes* |
| H42027f_a01 | TrAa01ScC | CH3CHOHOOH $\rightarrow$ CH3CHOHOOH(aq) | k_exf(01,ind_CH3CHOHOOH) | see general notes* |
| H42027b_a01 | TrAa01ScC | CH3CHOHOOH(aq) $\rightarrow$ CH3CHOHOOH | k_exb(01,ind_CH3CHOHOOH) | see general notes* |
| H42028f_a01 | TrAa01ScCN | ETHOHNO3 $\rightarrow$ ETHOHNO3(aq) | k_exf(01,ind_ETHOHNO3) | see general notes* |
| H42028b_a01 | TrAa01ScCN | ETHOHNO3(aq) $\rightarrow$ ETHOHNO3 | k_exb(01,ind_ETHOHNO3) | see general notes* |
| H42029f_a01 | TrAa01ScC | $HCOCO_3H \rightarrow HCOCO_3H(aq)$ | k_exf(01,ind_HCOCO3H) | see general notes* |
| H42029b_a01 | TrAa01ScC | $HCOCO_3H(aq) \rightarrow HCOCO_3H$ | k_exb(01,ind_HCOCO3H) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H42030f_a01 | TrAa01ScC | HOOCH2CO3H → HOOCH2CO3H(aq) | k_exf(01,ind_HOOCH2CO3H) | see general notes* |
| H42030b_a01 | TrAa01ScC | HOOCH2CO3H(aq) → HOOCH2CO3H | k_exb(01,ind_HOOCH2CO3H) | see general notes* |
| H42031f_a01 | TrAa01ScC | HYETHO2H → HYETHO2H(aq) | k_exf(01,ind_HYETHO2H) | see general notes* |
| H42031b_a01 | TrAa01ScC | HYETHO2H(aq) → HYETHO2H | k_exb(01,ind_HYETHO2H) | see general notes* |
| H42032f_a01 | TrAa01ScCN | PHAN → PHAN(aq) | k_exf(01,ind_PHAN) | see general notes* |
| H42032b_a01 | TrAa01ScCN | PHAN(aq) → PHAN | k_exb(01,ind_PHAN) | see general notes* |
| H43000f_a01 | TrAa01ScC | $CH_3COCH_3$ → $CH_3COCH_3$(aq) | k_exf(01,ind_CH3COCH3) | see general notes* |
| H43000b_a01 | TrAa01ScC | $CH_3COCH_3$(aq) → $CH_3COCH_3$ | k_exb(01,ind_CH3COCH3) | see general notes* |
| H43001f_a01 | TrAa01ScC | MGLYOX → $CH_3C(O)CHO$(aq) | k_exf(01,ind_MGLYOX) | see general notes* |
| H43001b_a01 | TrAa01ScC | $CH_3C(O)CHO$(aq) → MGLYOX | k_exb(01,ind_MGLYOX) | see general notes* |
| H43002f_a01 | TrAa01ScC | $CH_3COCO_2H$ → $CH_3COCOOH$(aq) | k_exf(01,ind_CH3COCO2H) | see general notes* |
| H43002b_a01 | TrAa01ScC | $CH_3COCOOH$(aq) → $CH_3COCO_2H$ | k_exb(01,ind_CH3COCO2H) | see general notes* |
| H43003f_a01 | TrAa01ScC | $CH_3COCHOHOH$ → $CH_3COCHOHOH$(aq) | k_exf(01,ind_CH3COCHOHOH) | see general notes* |
| H43003b_a01 | TrAa01ScC | $CH_3COCHOHOH$(aq) → $CH_3COCHOHOH$ | k_exb(01,ind_CH3COCHOHOH) | see general notes* |
| H43005f_a01 | TrAa01ScC | IPROPOL → IPROPOL(aq) | k_exf(01,ind_IPROPOL) | see general notes* |
| H43005b_a01 | TrAa01ScC | IPROPOL(aq) → IPROPOL | k_exb(01,ind_IPROPOL) | see general notes* |
| H43006f_a01 | TrAa01ScC | $CH_3COCH_2O_2H$ → $CH_3COCH_2O_2H$(aq) | k_exf(01,ind_HYPERACET) | see general notes* |
| H43006b_a01 | TrAa01ScC | $CH_3COCH_2O_2H$(aq) → $CH_3COCH_2O_2H$ | k_exb(01,ind_HYPERACET) | see general notes* |
| H43007f_a01 | TrAa01ScC | $iC_3H_7OOH$ → $iC_3H_7OOH$(aq) | k_exf(01,ind_IC3H7OOH) | see general notes* |
| H43007b_a01 | TrAa01ScC | $iC_3H_7OOH$(aq) → $iC_3H_7OOH$ | k_exb(01,ind_IC3H7OOH) | see general notes* |
| H43008f_a01 | TrAa01ScC | $HCOCOCH_2OOH$ → $HCOCOCH_2OOH$(aq) | k_exf(01,ind_ALCOCH2OOH) | see general notes* |
| H43008b_a01 | TrAa01ScC | $HCOCOCH_2OOH$(aq) → $HCOCOCH_2OOH$ | k_exb(01,ind_ALCOCH2OOH) | see general notes* |
| H43009f_a01 | TrAa01ScC | C32OH13CO → C32OH13CO(aq) | k_exf(01,ind_C32OH13CO) | see general notes* |
| H43009b_a01 | TrAa01ScC | C32OH13CO(aq) → C32OH13CO | k_exb(01,ind_C32OH13CO) | see general notes* |
| H43010f_a01 | TrAa01ScC | HCOCOCHO → HCOCOCHO(aq) | k_exf(01,ind_C33CO) | see general notes* |
| H43010b_a01 | TrAa01ScC | HCOCOCHO(aq) → HCOCOCHO | k_exb(01,ind_C33CO) | see general notes* |
| H43011f_a01 | TrAa01ScC | C3DIALOOH → C3DIALOOH(aq) | k_exf(01,ind_C3DIALOOH) | see general notes* |
| H43011b_a01 | TrAa01ScC | C3DIALOOH(aq) → C3DIALOOH | k_exb(01,ind_C3DIALOOH) | see general notes* |
| H43012f_a01 | TrAa01ScCN | $C_3PAN1$ → $C_3PAN1$(aq) | k_exf(01,ind_C3PAN1) | see general notes* |
| H43012b_a01 | TrAa01ScCN | $C_3PAN1$(aq) → $C_3PAN1$ | k_exb(01,ind_C3PAN1) | see general notes* |
| H43013f_a01 | TrAa01ScCN | $C_3PAN2$ → $C_3PAN2$(aq) | k_exf(01,ind_C3PAN2) | see general notes* |
| H43013b_a01 | TrAa01ScCN | $C_3PAN2$(aq) → $C_3PAN2$ | k_exb(01,ind_C3PAN2) | see general notes* |
| H43014f_a01 | TrAa01ScC | CH3CHCO → CH3CHCO(aq) | k_exf(01,ind_CH3CHCO) | see general notes* |
| H43014b_a01 | TrAa01ScC | CH3CHCO(aq) → CH3CHCO | k_exb(01,ind_CH3CHCO) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H43015f_a01 | TrAa01ScCN | $CH_3COCH_2OONO_2 \rightarrow CH_3COCH_2OONO_2(aq)$ | k_exf(01,ind_CH3COCH2O2NO2) | see general notes* |
| H43015b_a01 | TrAa01ScCN | $CH_3COCH_2OONO_2(aq) \rightarrow CH_3COCH_2OONO_2$ | k_exb(01,ind_CH3COCH2O2NO2) | see general notes* |
| H43016f_a01 | TrAa01ScC | $CH_3COCO_3H \rightarrow CH_3COCO_3H(aq)$ | k_exf(01,ind_CH3COCO3H) | see general notes* |
| H43016b_a01 | TrAa01ScC | $CH_3COCO_3H(aq) \rightarrow CH_3COCO_3H$ | k_exb(01,ind_CH3COCO3H) | see general notes* |
| H43017f_a01 | TrAa01ScC | HCOCH2CHO → HCOCH2CHO(aq) | k_exf(01,ind_HCOCH2CHO) | see general notes* |
| H43017b_a01 | TrAa01ScC | HCOCH2CHO(aq) → HCOCH2CHO | k_exb(01,ind_HCOCH2CHO) | see general notes* |
| H43018f_a01 | TrAa01ScC | HCOCH2CO2H → HCOCH2CO2H(aq) | k_exf(01,ind_HCOCH2CO2H) | see general notes* |
| H43018b_a01 | TrAa01ScC | HCOCH2CO2H(aq) → HCOCH2CO2H | k_exb(01,ind_HCOCH2CO2H) | see general notes* |
| H43019f_a01 | TrAa01ScC | HCOCH2CO3H → HCOCH2CO3H(aq) | k_exf(01,ind_HCOCH2CO3H) | see general notes* |
| H43019b_a01 | TrAa01ScC | HCOCH2CO3H(aq) → HCOCH2CO3H | k_exb(01,ind_HCOCH2CO3H) | see general notes* |
| H43020f_a01 | TrAa01ScC | $HCOCOCH_2OOH \rightarrow HCOCOCH_2OOH(aq)$ | k_exf(01,ind_HCOCOCH2OOH) | see general notes* |
| H43020b_a01 | TrAa01ScC | $HCOCOCH_2OOH(aq) \rightarrow HCOCOCH_2OOH$ | k_exb(01,ind_HCOCOCH2OOH) | see general notes* |
| H43021f_a01 | TrAa01ScC | HCOCOHCO3H → HCOCOHCO3H(aq) | k_exf(01,ind_HCOCOHCO3H) | see general notes* |
| H43021b_a01 | TrAa01ScC | HCOCOHCO3H(aq) → HCOCOHCO3H | k_exb(01,ind_HCOCOHCO3H) | see general notes* |
| H43022f_a01 | TrAa01ScCN | HCOCOHPAN → HCOCOHPAN(aq) | k_exf(01,ind_HCOCOHPAN) | see general notes* |
| H43022b_a01 | TrAa01ScCN | HCOCOHPAN(aq) → HCOCOHPAN | k_exb(01,ind_HCOCOHPAN) | see general notes* |
| H43023f_a01 | TrAa01ScC | HOC2H4CO2H → HOC2H4CO2H(aq) | k_exf(01,ind_HOC2H4CO2H) | see general notes* |
| H43023b_a01 | TrAa01ScC | HOC2H4CO2H(aq) → HOC2H4CO2H | k_exb(01,ind_HOC2H4CO2H) | see general notes* |
| H43024f_a01 | TrAa01ScC | HOC2H4CO3H → HOC2H4CO3H(aq) | k_exf(01,ind_HOC2H4CO3H) | see general notes* |
| H43024b_a01 | TrAa01ScC | HOC2H4CO3H(aq) → HOC2H4CO3H | k_exb(01,ind_HOC2H4CO3H) | see general notes* |
| H43025f_a01 | TrAa01ScC | HOCH2COCH2OOH → HOCH2COCH2OOH(aq) | k_exf(01,ind_HOCH2COCH2OOH) | see general notes* |
| H43025b_a01 | TrAa01ScC | HOCH2COCH2OOH(aq) → HOCH2COCH2OOH | k_exb(01,ind_HOCH2COCH2OOH) | see general notes* |
| H43026f_a01 | TrAa01ScC | HOCH2COCHO → HOCH2COCHO(aq) | k_exf(01,ind_HOCH2COCHO) | see general notes* |
| H43026b_a01 | TrAa01ScC | HOCH2COCHO(aq) → HOCH2COCHO | k_exb(01,ind_HOCH2COCHO) | see general notes* |
| H43027f_a01 | TrAa01ScC | HYPROPO2H → HYPROPO2H(aq) | k_exf(01,ind_HYPROPO2H) | see general notes* |
| H43027b_a01 | TrAa01ScC | HYPROPO2H(aq) → HYPROPO2H | k_exb(01,ind_HYPROPO2H) | see general notes* |
| H43028f_a01 | TrAa01ScC | METACETHO → METACETHO(aq) | k_exf(01,ind_METACETHO) | see general notes* |
| H43028b_a01 | TrAa01ScC | METACETHO(aq) → METACETHO | k_exb(01,ind_METACETHO) | see general notes* |
| H43029f_a01 | TrAa01ScCN | NOA → NOA(aq) | k_exf(01,ind_NOA) | see general notes* |
| H43029b_a01 | TrAa01ScCN | NOA(aq) → NOA | k_exb(01,ind_NOA) | see general notes* |
| H43030f_a01 | TrAa01ScCN | PR2O2HNO3 → PR2O2HNO3(aq) | k_exf(01,ind_PR2O2HNO3) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H43030b_a01 | TrAa01ScCN | PR2O2HNO3(aq) → PR2O2HNO3 | k_exb(01,ind_PR2O2HNO3) | see general notes* |
| H43031f_a01 | TrAa01ScCN | PROPOLNO3 → PROPOLNO3(aq) | k_exf(01,ind_PROPOLNO3) | see general notes* |
| H43031b_a01 | TrAa01ScCN | PROPOLNO3(aq) → PROPOLNO3 | k_exb(01,ind_PROPOLNO3) | see general notes* |
| H43032f_a01 | TrAa01ScC | $CH_3COCH_2OH$ → $CH_3COCH_2OH$(aq) | k_exf(01,ind_ACETOL) | see general notes* |
| H43032b_a01 | TrAa01ScC | $CH_3COCH_2OH$(aq) → $CH_3COCH_2OH$ | k_exb(01,ind_ACETOL) | see general notes* |
| H44000f_a01 | TrAa01ScC | MACR → MACR(aq) | k_exf(01,ind_MACR) | see general notes* |
| H44000b_a01 | TrAa01ScC | MACR(aq) → MACR | k_exb(01,ind_MACR) | see general notes* |
| H44001f_a01 | TrAa01ScC | MVK → MVK(aq) | k_exf(01,ind_MVK) | see general notes* |
| H44001b_a01 | TrAa01ScC | MVK(aq) → MVK | k_exb(01,ind_MVK) | see general notes* |
| H44002f_a01 | TrAa01ScC | $CH_3COCOCH_2O_2$ → $CH_3COCOCH_2O_2$(aq) | k_exf(01,ind_BIACETO2) | see general notes* |
| H44002b_a01 | TrAa01ScC | $CH_3COCOCH_2O_2$(aq) → $CH_3COCOCH_2O_2$ | k_exb(01,ind_BIACETO2) | see general notes* |
| H44003f_a01 | TrAa01ScC | BIACETOH → BIACETOH(aq) | k_exf(01,ind_BIACETOH) | see general notes* |
| H44003b_a01 | TrAa01ScC | BIACETOH(aq) → BIACETOH | k_exb(01,ind_BIACETOH) | see general notes* |
| H44004f_a01 | TrAa01ScC | $CH_3COCOCH_2OOH$ → $CH_3COCOCH_2OOH$(aq) | k_exf(01,ind_BIACETOOH) | see general notes* |
| H44004b_a01 | TrAa01ScC | $CH_3COCOCH_2OOH$(aq) → $CH_3COCOCH_2OOH$ | k_exb(01,ind_BIACETOOH) | see general notes* |
| H44005f_a01 | TrAa01ScC | BUT2OLO → BUT2OLO(aq) | k_exf(01,ind_BUT2OLO) | see general notes* |
| H44005b_a01 | TrAa01ScC | BUT2OLO(aq) → BUT2OLO | k_exb(01,ind_BUT2OLO) | see general notes* |
| H44006f_a01 | TrAa01ScC | BUT2OLOOH → BUT2OLOOH(aq) | k_exf(01,ind_BUT2OLOOH) | see general notes* |
| H44006b_a01 | TrAa01ScC | BUT2OLOOH(aq) → BUT2OLOOH | k_exb(01,ind_BUT2OLOOH) | see general notes* |
| H44007f_a01 | TrAa01ScC | BZFUCO → BZFUCO(aq) | k_exf(01,ind_BZFUCO) | see general notes* |
| H44007b_a01 | TrAa01ScC | BZFUCO(aq) → BZFUCO | k_exb(01,ind_BZFUCO) | see general notes* |
| H44008f_a01 | TrAa01ScC | BZFUOOH → BZFUOOH(aq) | k_exf(01,ind_BZFUOOH) | see general notes* |
| H44008b_a01 | TrAa01ScC | BZFUOOH(aq) → BZFUOOH | k_exb(01,ind_BZFUOOH) | see general notes* |
| H44009f_a01 | TrAa01ScC | C312COCO3H → C312COCO3H(aq) | k_exf(01,ind_C312COCO3H) | see general notes* |
| H44009b_a01 | TrAa01ScC | C312COCO3H(aq) → C312COCO3H | k_exb(01,ind_C312COCO3H) | see general notes* |
| H44010f_a01 | TrAa01ScCN | C312COPAN → C312COPAN(aq) | k_exf(01,ind_C312COPAN) | see general notes* |
| H44010b_a01 | TrAa01ScCN | C312COPAN(aq) → C312COPAN | k_exb(01,ind_C312COPAN) | see general notes* |
| H44011f_a01 | TrAa01ScC | C413COOOH → C413COOOH(aq) | k_exf(01,ind_C413COOOH) | see general notes* |
| H44011b_a01 | TrAa01ScC | C413COOOH(aq) → C413COOOH | k_exb(01,ind_C413COOOH) | see general notes* |
| H44012f_a01 | TrAa01ScC | C44OOH → C44OOH(aq) | k_exf(01,ind_C44OOH) | see general notes* |
| H44012b_a01 | TrAa01ScC | C44OOH(aq) → C44OOH | k_exb(01,ind_C44OOH) | see general notes* |
| H44013f_a01 | TrAa01ScC | C4CODIAL → C4CODIAL(aq) | k_exf(01,ind_C4CODIAL) | see general notes* |
| H44013b_a01 | TrAa01ScC | C4CODIAL(aq) → C4CODIAL | k_exb(01,ind_C4CODIAL) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H44014f_a01 | TrAa01ScCN | C4PAN5 → C4PAN5(aq) | k_exf(01,ind_C4PAN5) | see general notes* |
| H44014b_a01 | TrAa01ScCN | C4PAN5(aq) → C4PAN5 | k_exb(01,ind_C4PAN5) | see general notes* |
| H44015f_a01 | TrAa01ScC | $CH_3COCHCO$ → $CH_3COCHCO(aq)$ | k_exf(01,ind_CH3COCHCO) | see general notes* |
| H44015b_a01 | TrAa01ScC | $CH_3COCHCO(aq)$ → $CH_3COCHCO$ | k_exb(01,ind_CH3COCHCO) | see general notes* |
| H44016f_a01 | TrAa01ScC | CH3COCOCO2H → CH3COCOCO2H(aq) | k_exf(01,ind_CH3COCOCO2H) | see general notes* |
| H44016b_a01 | TrAa01ScC | CH3COCOCO2H(aq) → CH3COCOCO2H | k_exb(01,ind_CH3COCOCO2H) | see general notes* |
| H44017f_a01 | TrAa01ScC | $CH_3COOHCHCHO$ → $CH_3COOHCHCHO(aq)$ | k_exf(01,ind_CH3COOHCHCHO) | see general notes* |
| H44017b_a01 | TrAa01ScC | $CH_3COOHCHCHO(aq)$ → $CH_3COOHCHCHO$ | k_exb(01,ind_CH3COOHCHCHO) | see general notes* |
| H44018f_a01 | TrAa01ScC | CHOC3COO2 → CHOC3COO2(aq) | k_exf(01,ind_CHOC3COO2) | see general notes* |
| H44018b_a01 | TrAa01ScC | CHOC3COO2(aq) → CHOC3COO2 | k_exb(01,ind_CHOC3COO2) | see general notes* |
| H44019f_a01 | TrAa01ScC | CO14O3CHO → CO14O3CHO(aq) | k_exf(01,ind_CO14O3CHO) | see general notes* |
| H44019b_a01 | TrAa01ScC | CO14O3CHO(aq) → CO14O3CHO | k_exb(01,ind_CO14O3CHO) | see general notes* |
| H44020f_a01 | TrAa01ScC | CO14O3CO2H → CO14O3CO2H(aq) | k_exf(01,ind_CO14O3CO2H) | see general notes* |
| H44020b_a01 | TrAa01ScC | CO14O3CO2H(aq) → CO14O3CO2H | k_exb(01,ind_CO14O3CO2H) | see general notes* |
| H44021f_a01 | TrAa01ScC | $CH_3COCOCHO$ → $CH_3COCOCHO(aq)$ | k_exf(01,ind_CO23C3CHO) | see general notes* |
| H44021b_a01 | TrAa01ScC | $CH_3COCOCHO(aq)$ → $CH_3COCOCHO$ | k_exb(01,ind_CO23C3CHO) | see general notes* |
| H44022f_a01 | TrAa01ScC | CO2C3CHO → CO2C3CHO(aq) | k_exf(01,ind_CO2C3CHO) | see general notes* |
| H44022b_a01 | TrAa01ScC | CO2C3CHO(aq) → CO2C3CHO | k_exb(01,ind_CO2C3CHO) | see general notes* |
| H44023f_a01 | TrAa01ScC | CO2C4DIAL → CO2C4DIAL(aq) | k_exf(01,ind_CO2C4DIAL) | see general notes* |
| H44023b_a01 | TrAa01ScC | CO2C4DIAL(aq) → CO2C4DIAL | k_exb(01,ind_CO2C4DIAL) | see general notes* |
| H44024f_a01 | TrAa01ScC | CO2H3CHO → CO2H3CHO(aq) | k_exf(01,ind_CO2H3CHO) | see general notes* |
| H44024b_a01 | TrAa01ScC | CO2H3CHO(aq) → CO2H3CHO | k_exb(01,ind_CO2H3CHO) | see general notes* |
| H44025f_a01 | TrAa01ScC | CO2H3CO2H → CO2H3CO2H(aq) | k_exf(01,ind_CO2H3CO2H) | see general notes* |
| H44025b_a01 | TrAa01ScC | CO2H3CO2H(aq) → CO2H3CO2H | k_exb(01,ind_CO2H3CO2H) | see general notes* |
| H44026f_a01 | TrAa01ScC | CO2H3CO3H → CO2H3CO3H(aq) | k_exf(01,ind_CO2H3CO3H) | see general notes* |
| H44026b_a01 | TrAa01ScC | CO2H3CO3H(aq) → CO2H3CO3H | k_exb(01,ind_CO2H3CO3H) | see general notes* |
| H44027f_a01 | TrAa01ScC | EPXC4DIAL → EPXC4DIAL(aq) | k_exf(01,ind_EPXC4DIAL) | see general notes* |
| H44027b_a01 | TrAa01ScC | EPXC4DIAL(aq) → EPXC4DIAL | k_exb(01,ind_EPXC4DIAL) | see general notes* |
| H44028f_a01 | TrAa01ScC | EPXDLCO2H → EPXDLCO2H(aq) | k_exf(01,ind_EPXDLCO2H) | see general notes* |
| H44028b_a01 | TrAa01ScC | EPXDLCO2H(aq) → EPXDLCO2H | k_exb(01,ind_EPXDLCO2H) | see general notes* |
| H44029f_a01 | TrAa01ScC | EPXDLCO3H → EPXDLCO3H(aq) | k_exf(01,ind_EPXDLCO3H) | see general notes* |
| H44029b_a01 | TrAa01ScC | EPXDLCO3H(aq) → EPXDLCO3H | k_exb(01,ind_EPXDLCO3H) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H44030f_a01 | TrAa01ScC | $HCOCCH_3CHOOH$ → $HCOCCH_3CHOOH(aq)$ | k_exf(01,ind_HCOCCH3CHOOH) | see general notes* |
| H44030b_a01 | TrAa01ScC | $HCOCCH_3CHOOH(aq)$ → $HCOCCH_3CHOOH$ | k_exb(01,ind_HCOCCH3CHOOH) | see general notes* |
| H44031f_a01 | TrAa01ScC | $HCOCCH_3CO$ → $HCOCCH_3CO(aq)$ | k_exf(01,ind_HCOCCH3CO) | see general notes* |
| H44031b_a01 | TrAa01ScC | $HCOCCH_3CO(aq)$ → $HCOCCH_3CO$ | k_exb(01,ind_HCOCCH3CO) | see general notes* |
| H44032f_a01 | TrAa01ScC | HMAC → HMAC(aq) | k_exf(01,ind_HMAC) | see general notes* |
| H44032b_a01 | TrAa01ScC | HMAC(aq) → HMAC | k_exb(01,ind_HMAC) | see general notes* |
| H44033f_a01 | TrAa01ScC | HO12CO3C4 → HO12CO3C4(aq) | k_exf(01,ind_HO12CO3C4) | see general notes* |
| H44033b_a01 | TrAa01ScC | HO12CO3C4(aq) → HO12CO3C4 | k_exb(01,ind_HO12CO3C4) | see general notes* |
| H44034f_a01 | TrAa01ScC | HOCOC4DIAL → HOCOC4DIAL(aq) | k_exf(01,ind_HOCOC4DIAL) | see general notes* |
| H44034b_a01 | TrAa01ScC | HOCOC4DIAL(aq) → HOCOC4DIAL | k_exb(01,ind_HOCOC4DIAL) | see general notes* |
| H44035f_a01 | TrAa01ScC | HVMK → HVMK(aq) | k_exf(01,ind_HVMK) | see general notes* |
| H44035b_a01 | TrAa01ScC | HVMK(aq) → HVMK | k_exb(01,ind_HVMK) | see general notes* |
| H44036f_a01 | TrAa01ScC | IBUTALOH → IBUTALOH(aq) | k_exf(01,ind_IBUTALOH) | see general notes* |
| H44036b_a01 | TrAa01ScC | IBUTALOH(aq) → IBUTALOH | k_exb(01,ind_IBUTALOH) | see general notes* |
| H44037f_a01 | TrAa01ScC | IBUTDIAL → IBUTDIAL(aq) | k_exf(01,ind_IBUTDIAL) | see general notes* |
| H44037b_a01 | TrAa01ScC | IBUTDIAL(aq) → IBUTDIAL | k_exb(01,ind_IBUTDIAL) | see general notes* |
| H44038f_a01 | TrAa01ScC | IBUTOLBOOH → IBUTOLBOOH(aq) | k_exf(01,ind_IBUTOLBOOH) | see general notes* |
| H44038b_a01 | TrAa01ScC | IBUTOLBOOH(aq) → IBUTOLBOOH | k_exb(01,ind_IBUTOLBOOH) | see general notes* |
| H44039f_a01 | TrAa01ScC | IPRHOCO2H → IPRHOCO2H(aq) | k_exf(01,ind_IPRHOCO2H) | see general notes* |
| H44039b_a01 | TrAa01ScC | IPRHOCO2H(aq) → IPRHOCO2H | k_exb(01,ind_IPRHOCO2H) | see general notes* |
| H44040f_a01 | TrAa01ScC | IPRHOCO3H → IPRHOCO3H(aq) | k_exf(01,ind_IPRHOCO3H) | see general notes* |
| H44040b_a01 | TrAa01ScC | IPRHOCO3H(aq) → IPRHOCO3H | k_exb(01,ind_IPRHOCO3H) | see general notes* |
| H44041f_a01 | TrAa01ScC | LBUT1ENOOH → LBUT1ENOOH(aq) | k_exf(01,ind_LBUT1ENOOH) | see general notes* |
| H44041b_a01 | TrAa01ScC | LBUT1ENOOH(aq) → LBUT1ENOOH | k_exb(01,ind_LBUT1ENOOH) | see general notes* |
| H44042f_a01 | TrAa01ScC | LHMVKABOOH → LHMVKABOOH(aq) | k_exf(01,ind_LHMVKABOOH) | see general notes* |
| H44042b_a01 | TrAa01ScC | LHMVKABOOH(aq) → LHMVKABOOH | k_exb(01,ind_LHMVKABOOH) | see general notes* |
| H44043f_a01 | TrAa01ScC | LMEKOOH → LMEKOOH(aq) | k_exf(01,ind_LMEKOOH) | see general notes* |
| H44043b_a01 | TrAa01ScC | LMEKOOH(aq) → LMEKOOH | k_exb(01,ind_LMEKOOH) | see general notes* |
| H44044f_a01 | TrAa01ScC | MACO2H → MACO2H(aq) | k_exf(01,ind_MACO2H) | see general notes* |
| H44044b_a01 | TrAa01ScC | MACO2H(aq) → MACO2H | k_exb(01,ind_MACO2H) | see general notes* |
| H44045f_a01 | TrAa01ScC | MACO3H → MACO3H(aq) | k_exf(01,ind_MACO3H) | see general notes* |
| H44045b_a01 | TrAa01ScC | MACO3H(aq) → MACO3H | k_exb(01,ind_MACO3H) | see general notes* |
| H44046f_a01 | TrAa01ScC | MACROH → MACROH(aq) | k_exf(01,ind_MACROH) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H44046b_a01 | TrAa01ScC | MACROH(aq) → MACROH | k_exb(01,ind_MACROH) | see general notes* |
| H44047f_a01 | TrAa01ScC | MACROOH → MACROOH(aq) | k_exf(01,ind_MACROOH) | see general notes* |
| H44047b_a01 | TrAa01ScC | MACROOH(aq) → MACROOH | k_exb(01,ind_MACROOH) | see general notes* |
| H44048f_a01 | TrAa01ScC | MALANHYOOH → MALANHYOOH(aq) | k_exf(01,ind_MALANHYOOH) | see general notes* |
| H44048b_a01 | TrAa01ScC | MALANHYOOH(aq) → MALANHYOOH | k_exb(01,ind_MALANHYOOH) | see general notes* |
| H44049f_a01 | TrAa01ScC | MALDALCO2H → MALDALCO2H(aq) | k_exf(01,ind_MALDALCO2H) | see general notes* |
| H44049b_a01 | TrAa01ScC | MALDALCO2H(aq) → MALDALCO2H | k_exb(01,ind_MALDALCO2H) | see general notes* |
| H44050f_a01 | TrAa01ScC | MALDALCO3H → MALDALCO3H(aq) | k_exf(01,ind_MALDALCO3H) | see general notes* |
| H44050b_a01 | TrAa01ScC | MALDALCO3H(aq) → MALDALCO3H | k_exb(01,ind_MALDALCO3H) | see general notes* |
| H44051f_a01 | TrAa01ScC | MALDIAL → MALDIAL(aq) | k_exf(01,ind_MALDIAL) | see general notes* |
| H44051b_a01 | TrAa01ScC | MALDIAL(aq) → MALDIAL | k_exb(01,ind_MALDIAL) | see general notes* |
| H44052f_a01 | TrAa01ScC | MALDIALOOH → MALDIALOOH(aq) | k_exf(01,ind_MALDIALOOH) | see general notes* |
| H44052b_a01 | TrAa01ScC | MALDIALOOH(aq) → MALDIALOOH | k_exb(01,ind_MALDIALOOH) | see general notes* |
| H44053f_a01 | TrAa01ScC | MALNHYOHCO → MALNHYOHCO(aq) | k_exf(01,ind_MALNHYOHCO) | see general notes* |
| H44053b_a01 | TrAa01ScC | MALNHYOHCO(aq) → MALNHYOHCO | k_exb(01,ind_MALNHYOHCO) | see general notes* |
| H44054f_a01 | TrAa01ScC | MECOACEOOH → MECOACEOOH(aq) | k_exf(01,ind_MECOACEOOH) | see general notes* |
| H44054b_a01 | TrAa01ScC | MECOACEOOH(aq) → MECOACEOOH | k_exb(01,ind_MECOACEOOH) | see general notes* |
| H44055f_a01 | TrAa01ScCN | MVKNO3 → MVKNO3(aq) | k_exf(01,ind_MVKNO3) | see general notes* |
| H44055b_a01 | TrAa01ScCN | MVKNO3(aq) → MVKNO3 | k_exb(01,ind_MVKNO3) | see general notes* |
| H44056f_a01 | TrAa01ScCN | NBZFUOOH → NBZFUOOH(aq) | k_exf(01,ind_NBZFUOOH) | see general notes* |
| H44056b_a01 | TrAa01ScCN | NBZFUOOH(aq) → NBZFUOOH | k_exb(01,ind_NBZFUOOH) | see general notes* |
| H44057f_a01 | TrAa01ScCN | NC4DCO2H → NC4DCO2H(aq) | k_exf(01,ind_NC4DCO2H) | see general notes* |
| H44057b_a01 | TrAa01ScCN | NC4DCO2H(aq) → NC4DCO2H | k_exb(01,ind_NC4DCO2H) | see general notes* |
| H45000f_a01 | TrAa01ScC | ACCOMECHO → ACCOMECHO(aq) | k_exf(01,ind_ACCOMECHO) | see general notes* |
| H45000b_a01 | TrAa01ScC | ACCOMECHO(aq) → ACCOMECHO | k_exb(01,ind_ACCOMECHO) | see general notes* |
| H45001f_a01 | TrAa01ScC | ACCOMECO3H → ACCOMECO3H(aq) | k_exf(01,ind_ACCOMECO3H) | see general notes* |
| H45001b_a01 | TrAa01ScC | ACCOMECO3H(aq) → ACCOMECO3H | k_exb(01,ind_ACCOMECO3H) | see general notes* |
| H45002f_a01 | TrAa01ScC | C1ODC2O2C4OOH → C1ODC2O2C4OOH(aq) | k_exf(01,ind_C1ODC2O2C4OOH) | see general notes* |
| H45002b_a01 | TrAa01ScC | C1ODC2O2C4OOH(aq) → C1ODC2O2C4OOH | k_exb(01,ind_C1ODC2O2C4OOH) | see general notes* |
| H45003f_a01 | TrAa01ScC | C1ODC2OOHC4OD → C1ODC2OOHC4OD(aq) | k_exf(01,ind_C1ODC2OOHC4OD) | see general notes* |
| H45003b_a01 | TrAa01ScC | C1ODC2OOHC4OD(aq) → C1ODC2OOHC4OD | k_exb(01,ind_C1ODC2OOHC4OD) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H45004f_a01 | TrAa01ScC | C1ODC3O2C4OOH → C1ODC3O2C4OOH(aq) | k_exf(01,ind_C1ODC3O2C4OOH) | see general notes* |
| H45004b_a01 | TrAa01ScC | C1ODC3O2C4OOH(aq) → C1ODC3O2C4OOH | k_exb(01,ind_C1ODC3O2C4OOH) | see general notes* |
| H45005f_a01 | TrAa01ScC | C1OOHC2OOHC4OD → C1OOHC2OOHC4OD(aq) | k_exf(01,ind_C1OOHC2OOHC4OD) | see general notes* |
| H45005b_a01 | TrAa01ScC | C1OOHC2OOHC4OD(aq) → C1OOHC2OOHC4OD | k_exb(01,ind_C1OOHC2OOHC4OD) | see general notes* |
| H45006f_a01 | TrAa01ScC | C24O3CCO2H → C24O3CCO2H(aq) | k_exf(01,ind_C24O3CCO2H) | see general notes* |
| H45006b_a01 | TrAa01ScC | C24O3CCO2H(aq) → C24O3CCO2H | k_exb(01,ind_C24O3CCO2H) | see general notes* |
| H45007f_a01 | TrAa01ScC | C4CO2DBCO3 → C4CO2DBCO3(aq) | k_exf(01,ind_C4CO2DBCO3) | see general notes* |
| H45007b_a01 | TrAa01ScC | C4CO2DBCO3(aq) → C4CO2DBCO3 | k_exb(01,ind_C4CO2DBCO3) | see general notes* |
| H45008f_a01 | TrAa01ScCN | C4CO2DBPAN → C4CO2DBPAN(aq) | k_exf(01,ind_C4CO2DBPAN) | see general notes* |
| H45008b_a01 | TrAa01ScCN | C4CO2DBPAN(aq) → C4CO2DBPAN | k_exb(01,ind_C4CO2DBPAN) | see general notes* |
| H45009f_a01 | TrAa01ScC | C4CO2DCO3H → C4CO2DCO3H(aq) | k_exf(01,ind_C4CO2DCO3H) | see general notes* |
| H45009b_a01 | TrAa01ScC | C4CO2DCO3H(aq) → C4CO2DCO3H | k_exb(01,ind_C4CO2DCO3H) | see general notes* |
| H45010f_a01 | TrAa01ScCN | C4MCONO3OH → C4MCONO3OH(aq) | k_exf(01,ind_C4MCONO3OH) | see general notes* |
| H45010b_a01 | TrAa01ScCN | C4MCONO3OH(aq) → C4MCONO3OH | k_exb(01,ind_C4MCONO3OH) | see general notes* |
| H45011f_a01 | TrAa01ScC | C511OOH → C511OOH(aq) | k_exf(01,ind_C511OOH) | see general notes* |
| H45011b_a01 | TrAa01ScC | C511OOH(aq) → C511OOH | k_exb(01,ind_C511OOH) | see general notes* |
| H45012f_a01 | TrAa01ScC | C512OOH → C512OOH(aq) | k_exf(01,ind_C512OOH) | see general notes* |
| H45012b_a01 | TrAa01ScC | C512OOH(aq) → C512OOH | k_exb(01,ind_C512OOH) | see general notes* |
| H45013f_a01 | TrAa01ScC | C5134CO2OH → C5134CO2OH(aq) | k_exf(01,ind_C5134CO2OH) | see general notes* |
| H45013b_a01 | TrAa01ScC | C5134CO2OH(aq) → C5134CO2OH | k_exb(01,ind_C5134CO2OH) | see general notes* |
| H45014f_a01 | TrAa01ScC | C513CO → C513CO(aq) | k_exf(01,ind_C513CO) | see general notes* |
| H45014b_a01 | TrAa01ScC | C513CO(aq) → C513CO | k_exb(01,ind_C513CO) | see general notes* |
| H45015f_a01 | TrAa01ScC | C513OOH → C513OOH(aq) | k_exf(01,ind_C513OOH) | see general notes* |
| H45015b_a01 | TrAa01ScC | C513OOH(aq) → C513OOH | k_exb(01,ind_C513OOH) | see general notes* |
| H45016f_a01 | TrAa01ScCN | C514NO3 → C514NO3(aq) | k_exf(01,ind_C514NO3) | see general notes* |
| H45016b_a01 | TrAa01ScCN | C514NO3(aq) → C514NO3 | k_exb(01,ind_C514NO3) | see general notes* |
| H45017f_a01 | TrAa01ScC | C514OOH → C514OOH(aq) | k_exf(01,ind_C514OOH) | see general notes* |
| H45017b_a01 | TrAa01ScC | C514OOH(aq) → C514OOH | k_exb(01,ind_C514OOH) | see general notes* |
| H45018f_a01 | TrAa01ScC | C54CO → C54CO(aq) | k_exf(01,ind_C54CO) | see general notes* |
| H45018b_a01 | TrAa01ScC | C54CO(aq) → C54CO | k_exb(01,ind_C54CO) | see general notes* |
| H45019f_a01 | TrAa01ScC | C59OOH → C59OOH(aq) | k_exf(01,ind_C59OOH) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H45019b_a01 | TrAa01ScC | C59OOH(aq) → C59OOH | k_exb(01,ind_C59OOH) | see general notes* |
| H45020f_a01 | TrAa01ScC | C5CO14OH → C5CO14OH(aq) | k_exf(01,ind_C5CO14OH) | see general notes* |
| H45020b_a01 | TrAa01ScC | C5CO14OH(aq) → C5CO14OH | k_exb(01,ind_C5CO14OH) | see general notes* |
| H45021f_a01 | TrAa01ScC | C5CO14OOH → C5CO14OOH(aq) | k_exf(01,ind_C5CO14OOH) | see general notes* |
| H45021b_a01 | TrAa01ScC | C5CO14OOH(aq) → C5CO14OOH | k_exb(01,ind_C5CO14OOH) | see general notes* |
| H45022f_a01 | TrAa01ScC | C5DIALCO → C5DIALCO(aq) | k_exf(01,ind_C5DIALCO) | see general notes* |
| H45022b_a01 | TrAa01ScC | C5DIALCO(aq) → C5DIALCO | k_exb(01,ind_C5DIALCO) | see general notes* |
| H45023f_a01 | TrAa01ScC | C5DIALOOH → C5DIALOOH(aq) | k_exf(01,ind_C5DIALOOH) | see general notes* |
| H45023b_a01 | TrAa01ScC | C5DIALOOH(aq) → C5DIALOOH | k_exb(01,ind_C5DIALOOH) | see general notes* |
| H45024f_a01 | TrAa01ScC | C5DICARB → C5DICARB(aq) | k_exf(01,ind_C5DICARB) | see general notes* |
| H45024b_a01 | TrAa01ScC | C5DICARB(aq) → C5DICARB | k_exb(01,ind_C5DICARB) | see general notes* |
| H45025f_a01 | TrAa01ScC | C5DICAROOH → C5DICAROOH(aq) | k_exf(01,ind_C5DICAROOH) | see general notes* |
| H45025b_a01 | TrAa01ScC | C5DICAROOH(aq) → C5DICAROOH | k_exb(01,ind_C5DICAROOH) | see general notes* |
| H45026f_a01 | TrAa01ScCN | C5PAN9 → C5PAN9(aq) | k_exf(01,ind_C5PAN9) | see general notes* |
| H45026b_a01 | TrAa01ScCN | C5PAN9(aq) → C5PAN9 | k_exb(01,ind_C5PAN9) | see general notes* |
| H45027f_a01 | TrAa01ScC | CHOC3COOOH → CHOC3COOOH(aq) | k_exf(01,ind_CHOC3COOOH) | see general notes* |
| H45027b_a01 | TrAa01ScC | CHOC3COOOH(aq) → CHOC3COOOH | k_exb(01,ind_CHOC3COOOH) | see general notes* |
| H45028f_a01 | TrAa01ScCN | CHOC3COPAN → CHOC3COPAN(aq) | k_exf(01,ind_CHOC3COPAN) | see general notes* |
| H45028b_a01 | TrAa01ScCN | CHOC3COPAN(aq) → CHOC3COPAN | k_exb(01,ind_CHOC3COPAN) | see general notes* |
| H45029f_a01 | TrAa01ScC | CO13C4CHO → CO13C4CHO(aq) | k_exf(01,ind_CO13C4CHO) | see general notes* |
| H45029b_a01 | TrAa01ScC | CO13C4CHO(aq) → CO13C4CHO | k_exb(01,ind_CO13C4CHO) | see general notes* |
| H45030f_a01 | TrAa01ScC | CO23C4CHO → CO23C4CHO(aq) | k_exf(01,ind_CO23C4CHO) | see general notes* |
| H45030b_a01 | TrAa01ScC | CO23C4CHO(aq) → CO23C4CHO | k_exb(01,ind_CO23C4CHO) | see general notes* |
| H45031f_a01 | TrAa01ScC | CO23C4CO3H → CO23C4CO3H(aq) | k_exf(01,ind_CO23C4CO3H) | see general notes* |
| H45031b_a01 | TrAa01ScC | CO23C4CO3H(aq) → CO23C4CO3H | k_exb(01,ind_CO23C4CO3H) | see general notes* |
| H45032f_a01 | TrAa01ScCN | DB1NO3 → DB1NO3(aq) | k_exf(01,ind_DB1NO3) | see general notes* |
| H45032b_a01 | TrAa01ScCN | DB1NO3(aq) → DB1NO3 | k_exb(01,ind_DB1NO3) | see general notes* |
| H45033f_a01 | TrAa01ScC | DB1OOH → DB1OOH(aq) | k_exf(01,ind_DB1OOH) | see general notes* |
| H45033b_a01 | TrAa01ScC | DB1OOH(aq) → DB1OOH | k_exb(01,ind_DB1OOH) | see general notes* |
| H45034f_a01 | TrAa01ScC | DB2OOH → DB2OOH(aq) | k_exf(01,ind_DB2OOH) | see general notes* |
| H45034b_a01 | TrAa01ScC | DB2OOH(aq) → DB2OOH | k_exb(01,ind_DB2OOH) | see general notes* |
| H45035f_a01 | TrAa01ScC | ISOPAOH → ISOPAOH(aq) | k_exf(01,ind_ISOPAOH) | see general notes* |
| H45035b_a01 | TrAa01ScC | ISOPAOH(aq) → ISOPAOH | k_exb(01,ind_ISOPAOH) | see general notes* |
| H45036f_a01 | TrAa01ScCN | ISOPBNO3 → ISOPBNO3(aq) | k_exf(01,ind_ISOPBNO3) | see general notes* |
| H45036b_a01 | TrAa01ScCN | ISOPBNO3(aq) → ISOPBNO3 | k_exb(01,ind_ISOPBNO3) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H45037f_a01 | TrAa01ScC | ISOPBOH → ISOPBOH(aq) | k_exf(01,ind_ISOPBOH) | see general notes* |
| H45037b_a01 | TrAa01ScC | ISOPBOH(aq) → ISOPBOH | k_exb(01,ind_ISOPBOH) | see general notes* |
| H45038f_a01 | TrAa01ScC | ISOPBOOH → ISOPBOOH(aq) | k_exf(01,ind_ISOPBOOH) | see general notes* |
| H45038b_a01 | TrAa01ScC | ISOPBOOH(aq) → ISOPBOOH | k_exb(01,ind_ISOPBOOH) | see general notes* |
| H45039f_a01 | TrAa01ScCN | ISOPDNO3 → ISOPDNO3(aq) | k_exf(01,ind_ISOPDNO3) | see general notes* |
| H45039b_a01 | TrAa01ScCN | ISOPDNO3(aq) → ISOPDNO3 | k_exb(01,ind_ISOPDNO3) | see general notes* |
| H45040f_a01 | TrAa01ScC | ISOPDOH → ISOPDOH(aq) | k_exf(01,ind_ISOPDOH) | see general notes* |
| H45040b_a01 | TrAa01ScC | ISOPDOH(aq) → ISOPDOH | k_exb(01,ind_ISOPDOH) | see general notes* |
| H45041f_a01 | TrAa01ScC | ISOPDOOH → ISOPDOOH(aq) | k_exf(01,ind_ISOPDOOH) | see general notes* |
| H45041b_a01 | TrAa01ScC | ISOPDOOH(aq) → ISOPDOOH | k_exb(01,ind_ISOPDOOH) | see general notes* |
| H45042f_a01 | TrAa01ScC | LC578OOH → LC578OOH(aq) | k_exf(01,ind_LC578OOH) | see general notes* |
| H45042b_a01 | TrAa01ScC | LC578OOH(aq) → LC578OOH | k_exb(01,ind_LC578OOH) | see general notes* |
| H45043f_a01 | TrAa01ScCN | LC5PAN1719 → LC5PAN1719(aq) | k_exf(01,ind_LC5PAN1719) | see general notes* |
| H45043b_a01 | TrAa01ScCN | LC5PAN1719(aq) → LC5PAN1719 | k_exb(01,ind_LC5PAN1719) | see general notes* |
| H45044f_a01 | TrAa01ScC | LHC4ACCHO → LHC4ACCHO(aq) | k_exf(01,ind_LHC4ACCHO) | see general notes* |
| H45044b_a01 | TrAa01ScC | LHC4ACCHO(aq) → LHC4ACCHO | k_exb(01,ind_LHC4ACCHO) | see general notes* |
| H45045f_a01 | TrAa01ScC | LHC4ACCO2H → LHC4ACCO2H(aq) | k_exf(01,ind_LHC4ACCO2H) | see general notes* |
| H45045b_a01 | TrAa01ScC | LHC4ACCO2H(aq) → LHC4ACCO2H | k_exb(01,ind_LHC4ACCO2H) | see general notes* |
| H45046f_a01 | TrAa01ScC | LHC4ACCO3H → LHC4ACCO3H(aq) | k_exf(01,ind_LHC4ACCO3H) | see general notes* |
| H45046b_a01 | TrAa01ScC | LHC4ACCO3H(aq) → LHC4ACCO3H | k_exb(01,ind_LHC4ACCO3H) | see general notes* |
| H45047f_a01 | TrAa01ScC | LIEPOX → LIEPOX(aq) | k_exf(01,ind_LIEPOX) | see general notes* |
| H45047b_a01 | TrAa01ScC | LIEPOX(aq) → LIEPOX | k_exb(01,ind_LIEPOX) | see general notes* |
| H45048f_a01 | TrAa01ScCN | LISOPACNO3 → LISOPACNO3(aq) | k_exf(01,ind_LISOPACNO3) | see general notes* |
| H45048b_a01 | TrAa01ScCN | LISOPACNO3(aq) → LISOPACNO3 | k_exb(01,ind_LISOPACNO3) | see general notes* |
| H45049f_a01 | TrAa01ScC | LISOPACOOH → LISOPACOOH(aq) | k_exf(01,ind_LISOPACOOH) | see general notes* |
| H45049b_a01 | TrAa01ScC | LISOPACOOH(aq) → LISOPACOOH | k_exb(01,ind_LISOPACOOH) | see general notes* |
| H45050f_a01 | TrAa01ScCN | LMBOABNO3 → LMBOABNO3(aq) | k_exf(01,ind_LMBOABNO3) | see general notes* |
| H45050b_a01 | TrAa01ScCN | LMBOABNO3(aq) → LMBOABNO3 | k_exb(01,ind_LMBOABNO3) | see general notes* |
| H45051f_a01 | TrAa01ScC | LMBOABOOH → LMBOABOOH(aq) | k_exf(01,ind_LMBOABOOH) | see general notes* |
| H45051b_a01 | TrAa01ScC | LMBOABOOH(aq) → LMBOABOOH | k_exb(01,ind_LMBOABOOH) | see general notes* |
| H45052f_a01 | TrAa01ScCN | LNMBOABOOH → LNMBOABOOH(aq) | k_exf(01,ind_LNMBOABOOH) | see general notes* |
| H45052b_a01 | TrAa01ScCN | LNMBOABOOH(aq) → LNMBOABOOH | k_exb(01,ind_LNMBOABOOH) | see general notes* |
| H45053f_a01 | TrAa01ScC | MBO → MBO(aq) | k_exf(01,ind_MBO) | see general notes* |
| H45053b_a01 | TrAa01ScC | MBO(aq) → MBO | k_exb(01,ind_MBO) | see general notes* |
| H45054f_a01 | TrAa01ScC | MBOACO → MBOACO(aq) | k_exf(01,ind_MBOACO) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H45054b_a01 | TrAa01ScC | MBOACO(aq) → MBOACO | k_exb(01,ind_MBOACO) | see general notes* |
| H45055f_a01 | TrAa01ScC | MBOCOCO → MBOCOCO(aq) | k_exf(01,ind_MBOCOCO) | see general notes* |
| H45055b_a01 | TrAa01ScC | MBOCOCO(aq) → MBOCOCO | k_exb(01,ind_MBOCOCO) | see general notes* |
| H45056f_a01 | TrAa01ScC | MC3ODBCO2H → MC3ODBCO2H(aq) | k_exf(01,ind_MC3ODBCO2H) | see general notes* |
| H45056b_a01 | TrAa01ScC | MC3ODBCO2H(aq) → MC3ODBCO2H | k_exb(01,ind_MC3ODBCO2H) | see general notes* |
| H45057f_a01 | TrAa01ScC | 3METHYLFURAN → 3METHYLFURAN(aq) | k_exf(01,ind_ME3FURAN) | see general notes* |
| H45057b_a01 | TrAa01ScC | 3METHYLFURAN(aq) → 3METHYLFURAN | k_exb(01,ind_ME3FURAN) | see general notes* |
| H45058f_a01 | TrAa01ScC | MMALNHYOOH → MMALNHYOOH(aq) | k_exf(01,ind_MMALNHYOOH) | see general notes* |
| H45058b_a01 | TrAa01ScC | MMALNHYOOH(aq) → MMALNHYOOH | k_exb(01,ind_MMALNHYOOH) | see general notes* |
| H45059f_a01 | TrAa01ScCN | NC4MDCO2HN → NC4MDCO2HN(aq) | k_exf(01,ind_NC4MDCO2H) | see general notes* |
| H45059b_a01 | TrAa01ScCN | NC4MDCO2HN(aq) → NC4MDCO2HN | k_exb(01,ind_NC4MDCO2H) | see general notes* |
| H45060f_a01 | TrAa01ScCN | NC4OHCO3H → NC4OHCO3H(aq) | k_exf(01,ind_NC4OHCO3H) | see general notes* |
| H45060b_a01 | TrAa01ScCN | NC4OHCO3H(aq) → NC4OHCO3H | k_exb(01,ind_NC4OHCO3H) | see general notes* |
| H45061f_a01 | TrAa01ScCN | NC4OHCPAN → NC4OHCPAN(aq) | k_exf(01,ind_NC4OHCPAN) | see general notes* |
| H45061b_a01 | TrAa01ScCN | NC4OHCPAN(aq) → NC4OHCPAN | k_exb(01,ind_NC4OHCPAN) | see general notes* |
| H45062f_a01 | TrAa01ScCN | NISOPOOH → NISOPOOH(aq) | k_exf(01,ind_NISOPOOH) | see general notes* |
| H45062b_a01 | TrAa01ScCN | NISOPOOH(aq) → NISOPOOH | k_exb(01,ind_NISOPOOH) | see general notes* |
| H45063f_a01 | TrAa01ScCN | NMBOBCO → NMBOBCO(aq) | k_exf(01,ind_NMBOBCO) | see general notes* |
| H45063b_a01 | TrAa01ScCN | NMBOBCO(aq) → NMBOBCO | k_exb(01,ind_NMBOBCO) | see general notes* |
| H45064f_a01 | TrAa01ScCN | NTLFUOOH → NTLFUOOH(aq) | k_exf(01,ind_NTLFUOOH) | see general notes* |
| H45064b_a01 | TrAa01ScCN | NTLFUOOH(aq) → NTLFUOOH | k_exb(01,ind_NTLFUOOH) | see general notes* |
| H45065f_a01 | TrAa01ScC | TLFUOOH → TLFUOOH(aq) | k_exf(01,ind_TLFUOOH) | see general notes* |
| H45065b_a01 | TrAa01ScC | TLFUOOH(aq) → TLFUOOH | k_exb(01,ind_TLFUOOH) | see general notes* |
| H45066f_a01 | TrAa01ScC | LZCO3HC23DBCOD → LZCO3HC23DBCOD(aq) | k_exf(01,ind_LZCO3HC23DBCOD) | see general notes* |
| H45066b_a01 | TrAa01ScC | LZCO3HC23DBCOD(aq) → LZCO3HC23DBCOD | k_exb(01,ind_LZCO3HC23DBCOD) | see general notes* |
| H45067f_a01 | TrAa01ScC | C4MDIAL → C4MDIAL(aq) | k_exf(01,ind_C4MDIAL) | see general notes* |
| H45067b_a01 | TrAa01ScC | C4MDIAL(aq) → C4MDIAL | k_exb(01,ind_C4MDIAL) | see general notes* |
| H46000f_a01 | TrAa01ScCN | BZBIPERNO3 → BZBIPERNO3(aq) | k_exf(01,ind_BZBIPERNO3) | see general notes* |
| H46000b_a01 | TrAa01ScCN | BZBIPERNO3(aq) → BZBIPERNO3 | k_exb(01,ind_BZBIPERNO3) | see general notes* |
| H46001f_a01 | TrAa01ScC | BZBIPEROOH → BZBIPEROOH(aq) | k_exf(01,ind_BZBIPEROOH) | see general notes* |
| H46001b_a01 | TrAa01ScC | BZBIPEROOH(aq) → BZBIPEROOH | k_exb(01,ind_BZBIPEROOH) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H46002f_a01 | TrAa01ScC | BZEMUCCO → BZEMUCCO(aq) | k_exf(01,ind_BZEMUCCO) | see general notes* |
| H46002b_a01 | TrAa01ScC | BZEMUCCO(aq) → BZEMUCCO | k_exb(01,ind_BZEMUCCO) | see general notes* |
| H46003f_a01 | TrAa01ScC | BZEMUCCO2H → BZEMUCCO2H(aq) | k_exf(01,ind_BZEMUCCO2H) | see general notes* |
| H46003b_a01 | TrAa01ScC | BZEMUCCO2H(aq) → BZEMUCCO2H | k_exb(01,ind_BZEMUCCO2H) | see general notes* |
| H46004f_a01 | TrAa01ScC | BZEMUCCO3H → BZEMUCCO3H(aq) | k_exf(01,ind_BZEMUCCO3H) | see general notes* |
| H46004b_a01 | TrAa01ScC | BZEMUCCO3H(aq) → BZEMUCCO3H | k_exb(01,ind_BZEMUCCO3H) | see general notes* |
| H46005f_a01 | TrAa01ScCN | BZEMUCNO3 → BZEMUCNO3(aq) | k_exf(01,ind_BZEMUCNO3) | see general notes* |
| H46005b_a01 | TrAa01ScCN | BZEMUCNO3(aq) → BZEMUCNO3 | k_exb(01,ind_BZEMUCNO3) | see general notes* |
| H46006f_a01 | TrAa01ScC | BZEMUCOOH → BZEMUCOOH(aq) | k_exf(01,ind_BZEMUCOOH) | see general notes* |
| H46006b_a01 | TrAa01ScC | BZEMUCOOH(aq) → BZEMUCOOH | k_exb(01,ind_BZEMUCOOH) | see general notes* |
| H46007f_a01 | TrAa01ScC | BZEPOXMUC → BZEPOXMUC(aq) | k_exf(01,ind_BZEPOXMUC) | see general notes* |
| H46007b_a01 | TrAa01ScC | BZEPOXMUC(aq) → BZEPOXMUC | k_exb(01,ind_BZEPOXMUC) | see general notes* |
| H46008f_a01 | TrAa01ScC | BZOBIPEROH → BZOBIPEROH(aq) | k_exf(01,ind_BZOBIPEROH) | see general notes* |
| H46008b_a01 | TrAa01ScC | BZOBIPEROH(aq) → BZOBIPEROH | k_exb(01,ind_BZOBIPEROH) | see general notes* |
| H46009f_a01 | TrAa01ScCN | C5CO2DBPAN → C5CO2DBPAN(aq) | k_exf(01,ind_C5CO2DBPAN) | see general notes* |
| H46009b_a01 | TrAa01ScCN | C5CO2DBPAN(aq) → C5CO2DBPAN | k_exb(01,ind_C5CO2DBPAN) | see general notes* |
| H46010f_a01 | TrAa01ScC | C5CO2DCO3H → C5CO2DCO3H(aq) | k_exf(01,ind_C5CO2DCO3H) | see general notes* |
| H46010b_a01 | TrAa01ScC | C5CO2DCO3H(aq) → C5CO2DCO3H | k_exb(01,ind_C5CO2DCO3H) | see general notes* |
| H46011f_a01 | TrAa01ScCN | C5CO2OHPAN → C5CO2OHPAN(aq) | k_exf(01,ind_C5CO2OHPAN) | see general notes* |
| H46011b_a01 | TrAa01ScCN | C5CO2OHPAN(aq) → C5CO2OHPAN | k_exb(01,ind_C5CO2OHPAN) | see general notes* |
| H46012f_a01 | TrAa01ScC | C5COOHCO3H → C5COOHCO3H(aq) | k_exf(01,ind_C5COOHCO3H) | see general notes* |
| H46012b_a01 | TrAa01ScC | C5COOHCO3H(aq) → C5COOHCO3H | k_exb(01,ind_C5COOHCO3H) | see general notes* |
| H46013f_a01 | TrAa01ScC | C6125CO → C6125CO(aq) | k_exf(01,ind_C6125CO) | see general notes* |
| H46013b_a01 | TrAa01ScC | C6125CO(aq) → C6125CO | k_exb(01,ind_C6125CO) | see general notes* |
| H46014f_a01 | TrAa01ScC | C614CO → C614CO(aq) | k_exf(01,ind_C614CO) | see general notes* |
| H46014b_a01 | TrAa01ScC | C614CO(aq) → C614CO | k_exb(01,ind_C614CO) | see general notes* |
| H46015f_a01 | TrAa01ScCN | C614NO3 → C614NO3(aq) | k_exf(01,ind_C614NO3) | see general notes* |
| H46015b_a01 | TrAa01ScCN | C614NO3(aq) → C614NO3 | k_exb(01,ind_C614NO3) | see general notes* |
| H46016f_a01 | TrAa01ScC | C614OOH → C614OOH(aq) | k_exf(01,ind_C614OOH) | see general notes* |
| H46016b_a01 | TrAa01ScC | C614OOH(aq) → C614OOH | k_exb(01,ind_C614OOH) | see general notes* |
| H46017f_a01 | TrAa01ScC | C615CO2OOH → C615CO2OOH(aq) | k_exf(01,ind_C615CO2OOH) | see general notes* |
| H46017b_a01 | TrAa01ScC | C615CO2OOH(aq) → C615CO2OOH | k_exb(01,ind_C615CO2OOH) | see general notes* |
| H46018f_a01 | TrAa01ScC | C6CO4DB → C6CO4DB(aq) | k_exf(01,ind_C6CO4DB) | see general notes* |
| H46018b_a01 | TrAa01ScC | C6CO4DB(aq) → C6CO4DB | k_exb(01,ind_C6CO4DB) | see general notes* |
| H46019f_a01 | TrAa01ScC | C6H5O → C6H5O(aq) | k_exf(01,ind_C6H5O) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H46019b_a01 | TrAa01ScC | C6H5O(aq) → C6H5O | k_exb(01,ind_C6H5O) | see general notes* |
| H46020f_a01 | TrAa01ScC | C6H5OOH → C6H5OOH(aq) | k_exf(01,ind_C6H5OOH) | see general notes* |
| H46020b_a01 | TrAa01ScC | C6H5OOH(aq) → C6H5OOH | k_exb(01,ind_C6H5OOH) | see general notes* |
| H46021f_a01 | TrAa01ScC | CATEC1O → CATEC1O(aq) | k_exf(01,ind_CATEC1O) | see general notes* |
| H46021b_a01 | TrAa01ScC | CATEC1O(aq) → CATEC1O | k_exb(01,ind_CATEC1O) | see general notes* |
| H46022f_a01 | TrAa01ScC | CATEC1OOH → CATEC1OOH(aq) | k_exf(01,ind_CATEC1OOH) | see general notes* |
| H46022b_a01 | TrAa01ScC | CATEC1OOH(aq) → CATEC1OOH | k_exb(01,ind_CATEC1OOH) | see general notes* |
| H46023f_a01 | TrAa01ScC | CATECHOL → CATECHOL(aq) | k_exf(01,ind_CATECHOL) | see general notes* |
| H46023b_a01 | TrAa01ScC | CATECHOL(aq) → CATECHOL | k_exb(01,ind_CATECHOL) | see general notes* |
| H46024f_a01 | TrAa01ScC | CO235C5CHO → CO235C5CHO(aq) | k_exf(01,ind_CO235C5CHO) | see general notes* |
| H46024b_a01 | TrAa01ScC | CO235C5CHO(aq) → CO235C5CHO | k_exb(01,ind_CO235C5CHO) | see general notes* |
| H46025f_a01 | TrAa01ScC | CO235C6OOH → CO235C6OOH(aq) | k_exf(01,ind_CO235C6OOH) | see general notes* |
| H46025b_a01 | TrAa01ScC | CO235C6OOH(aq) → CO235C6OOH | k_exb(01,ind_CO235C6OOH) | see general notes* |
| H46026f_a01 | TrAa01ScCN | DNPHEN → DNPHEN(aq) | k_exf(01,ind_DNPHEN) | see general notes* |
| H46026b_a01 | TrAa01ScCN | DNPHEN(aq) → DNPHEN | k_exb(01,ind_DNPHEN) | see general notes* |
| H46027f_a01 | TrAa01ScCN | DNPHENOOH → DNPHENOOH(aq) | k_exf(01,ind_DNPHENOOH) | see general notes* |
| H46027b_a01 | TrAa01ScCN | DNPHENOOH(aq) → DNPHENOOH | k_exb(01,ind_DNPHENOOH) | see general notes* |
| H46028f_a01 | TrAa01ScCN | NBZQOOH → NBZQOOH(aq) | k_exf(01,ind_NBZQOOH) | see general notes* |
| H46028b_a01 | TrAa01ScCN | NBZQOOH(aq) → NBZQOOH | k_exb(01,ind_NBZQOOH) | see general notes* |
| H46029f_a01 | TrAa01ScCN | NCATECHOL → NCATECHOL(aq) | k_exf(01,ind_NCATECHOL) | see general notes* |
| H46029b_a01 | TrAa01ScCN | NCATECHOL(aq) → NCATECHOL | k_exb(01,ind_NCATECHOL) | see general notes* |
| H46030f_a01 | TrAa01ScCN | NCATECOOH → NCATECOOH(aq) | k_exf(01,ind_NCATECOOH) | see general notes* |
| H46030b_a01 | TrAa01ScCN | NCATECOOH(aq) → NCATECOOH | k_exb(01,ind_NCATECOOH) | see general notes* |
| H46031f_a01 | TrAa01ScCN | NDNPHENOOH → NDNPHENOOH(aq) | k_exf(01,ind_NDNPHENOOH) | see general notes* |
| H46031b_a01 | TrAa01ScCN | NDNPHENOOH(aq) → NDNPHENOOH | k_exb(01,ind_NDNPHENOOH) | see general notes* |
| H46032f_a01 | TrAa01ScCN | NNCATECOOH → NNCATECOOH(aq) | k_exf(01,ind_NNCATECOOH) | see general notes* |
| H46032b_a01 | TrAa01ScCN | NNCATECOOH(aq) → NNCATECOOH | k_exb(01,ind_NNCATECOOH) | see general notes* |
| H46033f_a01 | TrAa01ScCN | NPHENOOH → NPHENOOH(aq) | k_exf(01,ind_NPHENOOH) | see general notes* |
| H46033b_a01 | TrAa01ScCN | NPHENOOH(aq) → NPHENOOH | k_exb(01,ind_NPHENOOH) | see general notes* |
| H46034f_a01 | TrAa01ScC | PBZQCO → PBZQCO(aq) | k_exf(01,ind_PBZQCO) | see general notes* |
| H46034b_a01 | TrAa01ScC | PBZQCO(aq) → PBZQCO | k_exb(01,ind_PBZQCO) | see general notes* |
| H46035f_a01 | TrAa01ScC | PBZQOOH → PBZQOOH(aq) | k_exf(01,ind_PBZQOOH) | see general notes* |
| H46035b_a01 | TrAa01ScC | PBZQOOH(aq) → PBZQOOH | k_exb(01,ind_PBZQOOH) | see general notes* |
| H46036f_a01 | TrAa01ScC | PHENOL → PHENOL(aq) | k_exf(01,ind_PHENOL) | see general notes* |
| H46036b_a01 | TrAa01ScC | PHENOL(aq) → PHENOL | k_exb(01,ind_PHENOL) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H46037f_a01 | TrAa01ScC | PHENOOH → PHENOOH(aq) | k_exf(01,ind_PHENOOH) | see general notes* |
| H46037b_a01 | TrAa01ScC | PHENOOH(aq) → PHENOOH | k_exb(01,ind_PHENOOH) | see general notes* |
| H47000f_a01 | TrAa01ScC | C235C6CO3H → C235C6CO3H(aq) | k_exf(01,ind_C235C6CO3H) | see general notes* |
| H47000b_a01 | TrAa01ScC | C235C6CO3H(aq) → C235C6CO3H | k_exb(01,ind_C235C6CO3H) | see general notes* |
| H47001f_a01 | TrAa01ScCN | C6CO2OHPAN → C6CO2OHPAN(aq) | k_exf(01,ind_C6CO2OHPAN) | see general notes* |
| H47001b_a01 | TrAa01ScCN | C6CO2OHPAN(aq) → C6CO2OHPAN | k_exb(01,ind_C6CO2OHPAN) | see general notes* |
| H47002f_a01 | TrAa01ScC | C6COOHCO3H → C6COOHCO3H(aq) | k_exf(01,ind_C6COOHCO3H) | see general notes* |
| H47002b_a01 | TrAa01ScC | C6COOHCO3H(aq) → C6COOHCO3H | k_exb(01,ind_C6COOHCO3H) | see general notes* |
| H47003f_a01 | TrAa01ScC | C6H5CH2OOH → C6H5CH2OOH(aq) | k_exf(01,ind_C6H5CH2OOH) | see general notes* |
| H47003b_a01 | TrAa01ScC | C6H5CH2OOH(aq) → C6H5CH2OOH | k_exb(01,ind_C6H5CH2OOH) | see general notes* |
| H47004f_a01 | TrAa01ScC | C6H5CO3H → C6H5CO3H(aq) | k_exf(01,ind_C6H5CO3H) | see general notes* |
| H47004b_a01 | TrAa01ScC | C6H5CO3H(aq) → C6H5CO3H | k_exb(01,ind_C6H5CO3H) | see general notes* |
| H47005f_a01 | TrAa01ScC | C716OOH → C716OOH(aq) | k_exf(01,ind_C716OOH) | see general notes* |
| H47005b_a01 | TrAa01ScC | C716OOH(aq) → C716OOH | k_exb(01,ind_C716OOH) | see general notes* |
| H47006f_a01 | TrAa01ScC | C721OOH → C721OOH(aq) | k_exf(01,ind_C721OOH) | see general notes* |
| H47006b_a01 | TrAa01ScC | C721OOH(aq) → C721OOH | k_exb(01,ind_C721OOH) | see general notes* |
| H47007f_a01 | TrAa01ScC | C722OOH → C722OOH(aq) | k_exf(01,ind_C722OOH) | see general notes* |
| H47007b_a01 | TrAa01ScC | C722OOH(aq) → C722OOH | k_exb(01,ind_C722OOH) | see general notes* |
| H47008f_a01 | TrAa01ScC | C7CO4DB → C7CO4DB(aq) | k_exf(01,ind_C7CO4DB) | see general notes* |
| H47008b_a01 | TrAa01ScC | C7CO4DB(aq) → C7CO4DB | k_exb(01,ind_C7CO4DB) | see general notes* |
| H47009f_a01 | TrAa01ScCN | C7PAN3 → C7PAN3(aq) | k_exf(01,ind_C7PAN3) | see general notes* |
| H47009b_a01 | TrAa01ScCN | C7PAN3(aq) → C7PAN3 | k_exb(01,ind_C7PAN3) | see general notes* |
| H47010f_a01 | TrAa01ScC | CO235C6CHO → CO235C6CHO(aq) | k_exf(01,ind_CO235C6CHO) | see general notes* |
| H47010b_a01 | TrAa01ScC | CO235C6CHO(aq) → CO235C6CHO | k_exb(01,ind_CO235C6CHO) | see general notes* |
| H47011f_a01 | TrAa01ScC | CRESOL → CRESOL(aq) | k_exf(01,ind_CRESOL) | see general notes* |
| H47011b_a01 | TrAa01ScC | CRESOL(aq) → CRESOL | k_exb(01,ind_CRESOL) | see general notes* |
| H47012f_a01 | TrAa01ScC | CRESOOH → CRESOOH(aq) | k_exf(01,ind_CRESOOH) | see general notes* |
| H47012b_a01 | TrAa01ScC | CRESOOH(aq) → CRESOOH | k_exb(01,ind_CRESOOH) | see general notes* |
| H47013f_a01 | TrAa01ScCN | DNCRES → DNCRES(aq) | k_exf(01,ind_DNCRES) | see general notes* |
| H47013b_a01 | TrAa01ScCN | DNCRES(aq) → DNCRES | k_exb(01,ind_DNCRES) | see general notes* |
| H47014f_a01 | TrAa01ScCN | DNCRESOOH → DNCRESOOH(aq) | k_exf(01,ind_DNCRESOOH) | see general notes* |
| H47014b_a01 | TrAa01ScCN | DNCRESOOH(aq) → DNCRESOOH | k_exb(01,ind_DNCRESOOH) | see general notes* |
| H47015f_a01 | TrAa01ScC | MCATEC1O → MCATEC1O(aq) | k_exf(01,ind_MCATEC1O) | see general notes* |
| H47015b_a01 | TrAa01ScC | MCATEC1O(aq) → MCATEC1O | k_exb(01,ind_MCATEC1O) | see general notes* |
| H47016f_a01 | TrAa01ScC | MCATEC1OOH → MCATEC1OOH(aq) | k_exf(01,ind_MCATEC1OOH) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H47016b_a01 | TrAa01ScC | MCATEC1OOH(aq) → MCATEC1OOH | k_exb(01,ind_MCATEC1OOH) | see general notes* |
| H47017f_a01 | TrAa01ScC | MCATECHOL → MCATECHOL(aq) | k_exf(01,ind_MCATECHOL) | see general notes* |
| H47017b_a01 | TrAa01ScC | MCATECHOL(aq) → MCATECHOL | k_exb(01,ind_MCATECHOL) | see general notes* |
| H47018f_a01 | TrAa01ScCN | MNCATECH → MNCATECH(aq) | k_exf(01,ind_MNCATECH) | see general notes* |
| H47018b_a01 | TrAa01ScCN | MNCATECH(aq) → MNCATECH | k_exb(01,ind_MNCATECH) | see general notes* |
| H47019f_a01 | TrAa01ScCN | MNCATECOOH → MNCATECOOH(aq) | k_exf(01,ind_MNCATECOOH) | see general notes* |
| H47019b_a01 | TrAa01ScCN | MNCATECOOH(aq) → MNCATECOOH | k_exb(01,ind_MNCATECOOH) | see general notes* |
| H47020f_a01 | TrAa01ScCN | MNNCATCOOH → MNNCATCOOH(aq) | k_exf(01,ind_MNNCATCOOH) | see general notes* |
| H47020b_a01 | TrAa01ScCN | MNNCATCOOH(aq) → MNNCATCOOH | k_exb(01,ind_MNNCATCOOH) | see general notes* |
| H47021f_a01 | TrAa01ScCN | NCRESOOH → NCRESOOH(aq) | k_exf(01,ind_NCRESOOH) | see general notes* |
| H47021b_a01 | TrAa01ScCN | NCRESOOH(aq) → NCRESOOH | k_exb(01,ind_NCRESOOH) | see general notes* |
| H47022f_a01 | TrAa01ScCN | NDNCRESOOH → NDNCRESOOH(aq) | k_exf(01,ind_NDNCRESOOH) | see general notes* |
| H47022b_a01 | TrAa01ScCN | NDNCRESOOH(aq) → NDNCRESOOH | k_exb(01,ind_NDNCRESOOH) | see general notes* |
| H47023f_a01 | TrAa01ScC | OXYL1OOH → OXYL1OOH(aq) | k_exf(01,ind_OXYL1OOH) | see general notes* |
| H47023b_a01 | TrAa01ScC | OXYL1OOH(aq) → OXYL1OOH | k_exb(01,ind_OXYL1OOH) | see general notes* |
| H47024f_a01 | TrAa01ScC | PHCOOH → PHCOOH(aq) | k_exf(01,ind_PHCOOH) | see general notes* |
| H47024b_a01 | TrAa01ScC | PHCOOH(aq) → PHCOOH | k_exb(01,ind_PHCOOH) | see general notes* |
| H47025f_a01 | TrAa01ScC | TLBIPEROOH → TLBIPEROOH(aq) | k_exf(01,ind_TLBIPEROOH) | see general notes* |
| H47025b_a01 | TrAa01ScC | TLBIPEROOH(aq) → TLBIPEROOH | k_exb(01,ind_TLBIPEROOH) | see general notes* |
| H47026f_a01 | TrAa01ScC | TLEMUCCO → TLEMUCCO(aq) | k_exf(01,ind_TLEMUCCO) | see general notes* |
| H47026b_a01 | TrAa01ScC | TLEMUCCO(aq) → TLEMUCCO | k_exb(01,ind_TLEMUCCO) | see general notes* |
| H47027f_a01 | TrAa01ScC | TLEMUCCO2H → TLEMUCCO2H(aq) | k_exf(01,ind_TLEMUCCO2H) | see general notes* |
| H47027b_a01 | TrAa01ScC | TLEMUCCO2H(aq) → TLEMUCCO2H | k_exb(01,ind_TLEMUCCO2H) | see general notes* |
| H47028f_a01 | TrAa01ScC | TLEMUCCO3H → TLEMUCCO3H(aq) | k_exf(01,ind_TLEMUCCO3H) | see general notes* |
| H47028b_a01 | TrAa01ScC | TLEMUCCO3H(aq) → TLEMUCCO3H | k_exb(01,ind_TLEMUCCO3H) | see general notes* |
| H47029f_a01 | TrAa01ScCN | TLEMUCNO3 → TLEMUCNO3(aq) | k_exf(01,ind_TLEMUCNO3) | see general notes* |
| H47029b_a01 | TrAa01ScCN | TLEMUCNO3(aq) → TLEMUCNO3 | k_exb(01,ind_TLEMUCNO3) | see general notes* |
| H47030f_a01 | TrAa01ScC | TLEMUCOOH → TLEMUCOOH(aq) | k_exf(01,ind_TLEMUCOOH) | see general notes* |
| H47030b_a01 | TrAa01ScC | TLEMUCOOH(aq) → TLEMUCOOH | k_exb(01,ind_TLEMUCOOH) | see general notes* |
| H47031f_a01 | TrAa01ScC | TLOBIPEROH → TLOBIPEROH(aq) | k_exf(01,ind_TLOBIPEROH) | see general notes* |
| H47031b_a01 | TrAa01ScC | TLOBIPEROH(aq) → TLOBIPEROH | k_exb(01,ind_TLOBIPEROH) | see general notes* |
| H47032f_a01 | TrAa01ScC | TOL1O → TOL1O(aq) | k_exf(01,ind_TOL1O) | see general notes* |
| H47032b_a01 | TrAa01ScC | TOL1O(aq) → TOL1O | k_exb(01,ind_TOL1O) | see general notes* |
| H48000f_a01 | TrAa01ScC | C721CHO → C721CHO(aq) | k_exf(01,ind_C721CHO) | see general notes* |
| H48000b_a01 | TrAa01ScC | C721CHO(aq) → C721CHO | k_exb(01,ind_C721CHO) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H48001f_a01 | TrAa01ScC | C721CO3H → C721CO3H(aq) | k_exf(01,ind_C721CO3H) | see general notes* |
| H48001b_a01 | TrAa01ScC | C721CO3H(aq) → C721CO3H | k_exb(01,ind_C721CO3H) | see general notes* |
| H48002f_a01 | TrAa01ScCN | C721PAN → C721PAN(aq) | k_exf(01,ind_C721PAN) | see general notes* |
| H48002b_a01 | TrAa01ScCN | C721PAN(aq) → C721PAN | k_exb(01,ind_C721PAN) | see general notes* |
| H48003f_a01 | TrAa01ScCN | C810NO3 → C810NO3(aq) | k_exf(01,ind_C810NO3) | see general notes* |
| H48003b_a01 | TrAa01ScCN | C810NO3(aq) → C810NO3 | k_exb(01,ind_C810NO3) | see general notes* |
| H48004f_a01 | TrAa01ScC | C810OOH → C810OOH(aq) | k_exf(01,ind_C810OOH) | see general notes* |
| H48004b_a01 | TrAa01ScC | C810OOH(aq) → C810OOH | k_exb(01,ind_C810OOH) | see general notes* |
| H48005f_a01 | TrAa01ScC | C812OOH → C812OOH(aq) | k_exf(01,ind_C812OOH) | see general notes* |
| H48005b_a01 | TrAa01ScC | C812OOH(aq) → C812OOH | k_exb(01,ind_C812OOH) | see general notes* |
| H48006f_a01 | TrAa01ScC | C813OOH → C813OOH(aq) | k_exf(01,ind_C813OOH) | see general notes* |
| H48006b_a01 | TrAa01ScC | C813OOH(aq) → C813OOH | k_exb(01,ind_C813OOH) | see general notes* |
| H48007f_a01 | TrAa01ScC | C85OOH → C85OOH(aq) | k_exf(01,ind_C85OOH) | see general notes* |
| H48007b_a01 | TrAa01ScC | C85OOH(aq) → C85OOH | k_exb(01,ind_C85OOH) | see general notes* |
| H48008f_a01 | TrAa01ScC | C86OOH → C86OOH(aq) | k_exf(01,ind_C86OOH) | see general notes* |
| H48008b_a01 | TrAa01ScC | C86OOH(aq) → C86OOH | k_exb(01,ind_C86OOH) | see general notes* |
| H48009f_a01 | TrAa01ScCN | C89NO3 → C89NO3(aq) | k_exf(01,ind_C89NO3) | see general notes* |
| H48009b_a01 | TrAa01ScCN | C89NO3(aq) → C89NO3 | k_exb(01,ind_C89NO3) | see general notes* |
| H48010f_a01 | TrAa01ScC | C89OOH → C89OOH(aq) | k_exf(01,ind_C89OOH) | see general notes* |
| H48010b_a01 | TrAa01ScC | C89OOH(aq) → C89OOH | k_exb(01,ind_C89OOH) | see general notes* |
| H48011f_a01 | TrAa01ScC | C8BC → C8BC(aq) | k_exf(01,ind_C8BC) | see general notes* |
| H48011b_a01 | TrAa01ScC | C8BC(aq) → C8BC | k_exb(01,ind_C8BC) | see general notes* |
| H48012f_a01 | TrAa01ScC | C8BCCO → C8BCCO(aq) | k_exf(01,ind_C8BCCO) | see general notes* |
| H48012b_a01 | TrAa01ScC | C8BCCO(aq) → C8BCCO | k_exb(01,ind_C8BCCO) | see general notes* |
| H48013f_a01 | TrAa01ScCN | C8BCNO3 → C8BCNO3(aq) | k_exf(01,ind_C8BCNO3) | see general notes* |
| H48013b_a01 | TrAa01ScCN | C8BCNO3(aq) → C8BCNO3 | k_exb(01,ind_C8BCNO3) | see general notes* |
| H48014f_a01 | TrAa01ScC | C8BCOOH → C8BCOOH(aq) | k_exf(01,ind_C8BCOOH) | see general notes* |
| H48014b_a01 | TrAa01ScC | C8BCOOH(aq) → C8BCOOH | k_exb(01,ind_C8BCOOH) | see general notes* |
| H48015f_a01 | TrAa01ScC | NORPINIC → NORPINIC(aq) | k_exf(01,ind_NORPINIC) | see general notes* |
| H48015b_a01 | TrAa01ScC | NORPINIC(aq) → NORPINIC | k_exb(01,ind_NORPINIC) | see general notes* |
| H48016f_a01 | TrAa01ScC | STYRENOOH → STYRENOOH(aq) | k_exf(01,ind_STYRENOOH) | see general notes* |
| H48016b_a01 | TrAa01ScC | STYRENOOH(aq) → STYRENOOH | k_exb(01,ind_STYRENOOH) | see general notes* |
| H49000f_a01 | TrAa01ScC | C811CO3H → C811CO3H(aq) | k_exf(01,ind_C811CO3H) | see general notes* |
| H49000b_a01 | TrAa01ScC | C811CO3H(aq) → C811CO3H | k_exb(01,ind_C811CO3H) | see general notes* |
| H49001f_a01 | TrAa01ScCN | C811PAN → C811PAN(aq) | k_exf(01,ind_C811PAN) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H49001b_a01 | TrAa01ScCN | C811PAN(aq) → C811PAN | k_exb(01,ind_C811PAN) | see general notes* |
| H49002f_a01 | TrAa01ScC | C85CO3H → C85CO3H(aq) | k_exf(01,ind_C85CO3H) | see general notes* |
| H49002b_a01 | TrAa01ScC | C85CO3H(aq) → C85CO3H | k_exb(01,ind_C85CO3H) | see general notes* |
| H49003f_a01 | TrAa01ScC | C89CO2H → C89CO2H(aq) | k_exf(01,ind_C89CO2H) | see general notes* |
| H49003b_a01 | TrAa01ScC | C89CO2H(aq) → C89CO2H | k_exb(01,ind_C89CO2H) | see general notes* |
| H49004f_a01 | TrAa01ScC | C89CO3H → C89CO3H(aq) | k_exf(01,ind_C89CO3H) | see general notes* |
| H49004b_a01 | TrAa01ScC | C89CO3H(aq) → C89CO3H | k_exb(01,ind_C89CO3H) | see general notes* |
| H49005f_a01 | TrAa01ScCN | C89PAN → C89PAN(aq) | k_exf(01,ind_C89PAN) | see general notes* |
| H49005b_a01 | TrAa01ScCN | C89PAN(aq) → C89PAN | k_exb(01,ind_C89PAN) | see general notes* |
| H49006f_a01 | TrAa01ScCN | C96NO3 → C96NO3(aq) | k_exf(01,ind_C96NO3) | see general notes* |
| H49006b_a01 | TrAa01ScCN | C96NO3(aq) → C96NO3 | k_exb(01,ind_C96NO3) | see general notes* |
| H49007f_a01 | TrAa01ScC | C96OOH → C96OOH(aq) | k_exf(01,ind_C96OOH) | see general notes* |
| H49007b_a01 | TrAa01ScC | C96OOH(aq) → C96OOH | k_exb(01,ind_C96OOH) | see general notes* |
| H49008f_a01 | TrAa01ScC | C97OOH → C97OOH(aq) | k_exf(01,ind_C97OOH) | see general notes* |
| H49008b_a01 | TrAa01ScC | C97OOH(aq) → C97OOH | k_exb(01,ind_C97OOH) | see general notes* |
| H49009f_a01 | TrAa01ScC | C98OOH → C98OOH(aq) | k_exf(01,ind_C98OOH) | see general notes* |
| H49009b_a01 | TrAa01ScC | C98OOH(aq) → C98OOH | k_exb(01,ind_C98OOH) | see general notes* |
| H49010f_a01 | TrAa01ScCN | C9PAN2 → C9PAN2(aq) | k_exf(01,ind_C9PAN2) | see general notes* |
| H49010b_a01 | TrAa01ScCN | C9PAN2(aq) → C9PAN2 | k_exb(01,ind_C9PAN2) | see general notes* |
| H49011f_a01 | TrAa01ScC | NOPINDCO → NOPINDCO(aq) | k_exf(01,ind_NOPINDCO) | see general notes* |
| H49011b_a01 | TrAa01ScC | NOPINDCO(aq) → NOPINDCO | k_exb(01,ind_NOPINDCO) | see general notes* |
| H49012f_a01 | TrAa01ScC | NOPINDOOH → NOPINDOOH(aq) | k_exf(01,ind_NOPINDOOH) | see general notes* |
| H49012b_a01 | TrAa01ScC | NOPINDOOH(aq) → NOPINDOOH | k_exb(01,ind_NOPINDOOH) | see general notes* |
| H49013f_a01 | TrAa01ScC | NOPINONE → NOPINONE(aq) | k_exf(01,ind_NOPINONE) | see general notes* |
| H49013b_a01 | TrAa01ScC | NOPINONE(aq) → NOPINONE | k_exb(01,ind_NOPINONE) | see general notes* |
| H49014f_a01 | TrAa01ScC | NOPINOO → NOPINOO(aq) | k_exf(01,ind_NOPINOO) | see general notes* |
| H49014b_a01 | TrAa01ScC | NOPINOO(aq) → NOPINOO | k_exb(01,ind_NOPINOO) | see general notes* |
| H49015f_a01 | TrAa01ScC | NORPINAL → NORPINAL(aq) | k_exf(01,ind_NORPINAL) | see general notes* |
| H49015b_a01 | TrAa01ScC | NORPINAL(aq) → NORPINAL | k_exb(01,ind_NORPINAL) | see general notes* |
| H49016f_a01 | TrAa01ScC | NORPINENOL → NORPINENOL(aq) | k_exf(01,ind_NORPINENOL) | see general notes* |
| H49016b_a01 | TrAa01ScC | NORPINENOL(aq) → NORPINENOL | k_exb(01,ind_NORPINENOL) | see general notes* |
| H49017f_a01 | TrAa01ScC | PINIC → PINIC(aq) | k_exf(01,ind_PINIC) | see general notes* |
| H49017b_a01 | TrAa01ScC | PINIC(aq) → PINIC | k_exb(01,ind_PINIC) | see general notes* |
| H410000f_a01 | TrAa01ScCN | BPINANO3 → BPINANO3(aq) | k_exf(01,ind_BPINANO3) | see general notes* |
| H410000b_a01 | TrAa01ScCN | BPINANO3(aq) → BPINANO3 | k_exb(01,ind_BPINANO3) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H410001f_a01 | TrAa01ScC | BPINAOOH → BPINAOOH(aq) | k_exf(01,ind_BPINAOOH) | see general notes* |
| H410001b_a01 | TrAa01ScC | BPINAOOH(aq) → BPINAOOH | k_exb(01,ind_BPINAOOH) | see general notes* |
| H410002f_a01 | TrAa01ScCN | C106NO3 → C106NO3(aq) | k_exf(01,ind_C106NO3) | see general notes* |
| H410002b_a01 | TrAa01ScCN | C106NO3(aq) → C106NO3 | k_exb(01,ind_C106NO3) | see general notes* |
| H410003f_a01 | TrAa01ScC | C106OOH → C106OOH(aq) | k_exf(01,ind_C106OOH) | see general notes* |
| H410003b_a01 | TrAa01ScC | C106OOH(aq) → C106OOH | k_exb(01,ind_C106OOH) | see general notes* |
| H410004f_a01 | TrAa01ScC | C109CO → C109CO(aq) | k_exf(01,ind_C109CO) | see general notes* |
| H410004b_a01 | TrAa01ScC | C109CO(aq) → C109CO | k_exb(01,ind_C109CO) | see general notes* |
| H410005f_a01 | TrAa01ScC | C109OOH → C109OOH(aq) | k_exf(01,ind_C109OOH) | see general notes* |
| H410005b_a01 | TrAa01ScC | C109OOH(aq) → C109OOH | k_exb(01,ind_C109OOH) | see general notes* |
| H410006f_a01 | TrAa01ScCN | C10PAN2 → C10PAN2(aq) | k_exf(01,ind_C10PAN2) | see general notes* |
| H410006b_a01 | TrAa01ScCN | C10PAN2(aq) → C10PAN2 | k_exb(01,ind_C10PAN2) | see general notes* |
| H410007f_a01 | TrAa01ScCN | LAPINABNO3 → LAPINABNO3(aq) | k_exf(01,ind_LAPINABNO3) | see general notes* |
| H410007b_a01 | TrAa01ScCN | LAPINABNO3(aq) → LAPINABNO3 | k_exb(01,ind_LAPINABNO3) | see general notes* |
| H410008f_a01 | TrAa01ScC | LAPINABOOH → LAPINABOOH(aq) | k_exf(01,ind_LAPINABOOH) | see general notes* |
| H410008b_a01 | TrAa01ScC | LAPINABOOH(aq) → LAPINABOOH | k_exb(01,ind_LAPINABOOH) | see general notes* |
| H410009f_a01 | TrAa01ScCN | LNAPINABOOH → LNAPINABOOH(aq) | k_exf(01,ind_LNAPINABOOH) | see general notes* |
| H410009b_a01 | TrAa01ScCN | LNAPINABOOH(aq) → LNAPINABOOH | k_exb(01,ind_LNAPINABOOH) | see general notes* |
| H410010f_a01 | TrAa01ScCN | LNBPINABOOH → LNBPINABOOH(aq) | k_exf(01,ind_LNBPINABOOH) | see general notes* |
| H410010b_a01 | TrAa01ScCN | LNBPINABOOH(aq) → LNBPINABOOH | k_exb(01,ind_LNBPINABOOH) | see general notes* |
| H410011f_a01 | TrAa01ScC | MENTHEN6ONE → MENTHEN6ONE(aq) | k_exf(01,ind_MENTHEN6ONE) | see general notes* |
| H410011b_a01 | TrAa01ScC | MENTHEN6ONE(aq) → MENTHEN6ONE | k_exb(01,ind_MENTHEN6ONE) | see general notes* |
| H410012f_a01 | TrAa01ScC | 2OHMENTHEN6ONE → 2OHMENTHEN6ONE(aq) | k_exf(01,ind_OH2MENTHEN6ONE) | see general notes* |
| H410012b_a01 | TrAa01ScC | 2OHMENTHEN6ONE(aq) → 2OHMENTHEN6ONE | k_exb(01,ind_OH2MENTHEN6ONE) | see general notes* |
| H410013f_a01 | TrAa01ScC | PERPINONIC → PERPINONIC(aq) | k_exf(01,ind_PERPINONIC) | see general notes* |
| H410013b_a01 | TrAa01ScC | PERPINONIC(aq) → PERPINONIC | k_exb(01,ind_PERPINONIC) | see general notes* |
| H410014f_a01 | TrAa01ScC | PINAL → PINAL(aq) | k_exf(01,ind_PINAL) | see general notes* |
| H410014b_a01 | TrAa01ScC | PINAL(aq) → PINAL | k_exb(01,ind_PINAL) | see general notes* |
| H410015f_a01 | TrAa01ScCN | PINALNO3 → PINALNO3(aq) | k_exf(01,ind_PINALNO3) | see general notes* |
| H410015b_a01 | TrAa01ScCN | PINALNO3(aq) → PINALNO3 | k_exb(01,ind_PINALNO3) | see general notes* |
| H410016f_a01 | TrAa01ScC | PINALOOH → PINALOOH(aq) | k_exf(01,ind_PINALOOH) | see general notes* |
| H410016b_a01 | TrAa01ScC | PINALOOH(aq) → PINALOOH | k_exb(01,ind_PINALOOH) | see general notes* |
| H410017f_a01 | TrAa01ScC | PINEOL → PINEOL(aq) | k_exf(01,ind_PINENOL) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H410017b_a01 | TrAa01ScC | PINEOL(aq) $\rightarrow$ PINEOL | k_exb(01,ind_PINENOL) | see general notes* |
| H410018f_a01 | TrAa01ScC | PINONIC $\rightarrow$ PINONIC(aq) | k_exf(01,ind_PINONIC) | see general notes* |
| H410018b_a01 | TrAa01ScC | PINONIC(aq) $\rightarrow$ PINONIC | k_exb(01,ind_PINONIC) | see general notes* |
| H410019f_a01 | TrAa01ScCN | RO6R1NO3 $\rightarrow$ RO6R1NO3(aq) | k_exf(01,ind_RO6R1NO3) | see general notes* |
| H410019b_a01 | TrAa01ScCN | RO6R1NO3(aq) $\rightarrow$ RO6R1NO3 | k_exb(01,ind_RO6R1NO3) | see general notes* |
| H410020f_a01 | TrAa01ScCN | ROO6R1NO3 $\rightarrow$ ROO6R1NO3(aq) | k_exf(01,ind_ROO6R1NO3) | see general notes* |
| H410020b_a01 | TrAa01ScCN | ROO6R1NO3(aq) $\rightarrow$ ROO6R1NO3 | k_exb(01,ind_ROO6R1NO3) | see general notes* |
| H60000f_a01 | TrAa01MblScCl | $Cl_2 \rightarrow Cl_2(aq)$ | k_exf(01,ind_Cl2) | see general notes* |
| H60000b_a01 | TrAa01MblScCl | $Cl_2(aq) \rightarrow Cl_2$ | k_exb(01,ind_Cl2) | see general notes* |
| H62000f_a01 | TrAa01MblScScmCl | $HCl \rightarrow HCl(aq)$ | k_exf(01,ind_HCl) | see general notes* |
| H62000b_a01 | TrAa01MblScScmCl | $HCl(aq) \rightarrow HCl$ | k_exb(01,ind_HCl) | see general notes* |
| H62001f_a01 | TrAa01MblScCl | $HOCl \rightarrow HOCl(aq)$ | k_exf(01,ind_HOCl) | see general notes* |
| H62001b_a01 | TrAa01MblScCl | $HOCl(aq) \rightarrow HOCl$ | k_exb(01,ind_HOCl) | see general notes* |
| H63000_a01 | TrAa01MblClN | $N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$ | k_exf_N2O5(01) * 5.E2 | Behnke et al. (1994), Behnke et al. (1997) |
| H63001_a01 | TrAa01MblClN | $ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$ | k_exf_ClNO3(01) * C(ind_H2O_a01) | see general notes* |
| H63002_a01 | TrAa01MblClN | $ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$ | k_exf_ClNO3(01) * 5.E2 | see general notes* |
| H70000f_a01 | TrAa01MblScBr | $Br_2 \rightarrow Br_2(aq)$ | k_exf(01,ind_Br2) | see general notes* |
| H70000b_a01 | TrAa01MblScBr | $Br_2(aq) \rightarrow Br_2$ | k_exb(01,ind_Br2) | see general notes* |
| H72000f_a01 | TrAa01MblScScmBr | $HBr \rightarrow HBr(aq)$ | k_exf(01,ind_HBr) | see general notes* |
| H72000b_a01 | TrAa01MblScScmBr | $HBr(aq) \rightarrow HBr$ | k_exb(01,ind_HBr) | see general notes* |
| H72001f_a01 | TrAa01MblScBr | $HOBr \rightarrow HOBr(aq)$ | k_exf(01,ind_HOBr) | see general notes* |
| H72001b_a01 | TrAa01MblScBr | $HOBr(aq) \rightarrow HOBr$ | k_exb(01,ind_HOBr) | see general notes* |
| H73000_a01 | TrAa01MblBrN | $N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$ | k_exf_N2O5(01) * 3.E5 | Behnke et al. (1994), Behnke et al. (1997) |
| H73001_a01 | TrAa01MblBrN | $BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$ | k_exf_BrNO3(01) * C(ind_H2O_a01) | see general notes* |
| H73002_a01 | TrAa01MblBrN | $BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$ | k_exf_BrNO3(01) * 3.E5 | see general notes* |
| H76000f_a01 | TrAa01MblScBrCl | $BrCl \rightarrow BrCl(aq)$ | k_exf(01,ind_BrCl) | see general notes* |
| H76000b_a01 | TrAa01MblScBrCl | $BrCl(aq) \rightarrow BrCl$ | k_exb(01,ind_BrCl) | see general notes* |
| H76001_a01 | TrAa01MblBrClN | $ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$ | k_exf_ClNO3(01) * 3.E5 | see general notes* |
| H76002_a01 | TrAa01MblBrClN | $BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$ | k_exf_BrNO3(01) * 5.E2 | see general notes* |
| H80000f_a01 | TrAa01ScI | $I_2 \rightarrow I_2(aq)$ | k_exf(01,ind_I2) | see general notes* |
| H80000b_a01 | TrAa01ScI | $I_2(aq) \rightarrow I_2$ | k_exb(01,ind_I2) | see general notes* |
| H81000f_a01 | TrAa01MblScI | $IO \rightarrow IO(aq)$ | k_exf(01,ind_IO) | see general notes* |

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| H81000b_a01 | TrAa01MblScI | IO(aq) $\rightarrow$ IO | k_exb(01,ind_IO) | see general notes* |
| H81001_a01 | TrAa01I | OIO $\rightarrow$ HOI(aq) + $HO_2$(aq) | k_exf(01,ind_OIO) | see general notes* |
| H81002_a01 | TrAa01I | $I_2O_2$ $\rightarrow$ HOI(aq) + $H^+$(aq) + $IO_2^-$(aq) | k_exf(01,ind_I2O2) | see general notes* |
| H82000f_a01 | TrAa01MblScI | HOI $\rightarrow$ HOI(aq) | k_exf(01,ind_HOI) | see general notes* |
| H82000b_a01 | TrAa01MblScI | HOI(aq) $\rightarrow$ HOI | k_exb(01,ind_HOI) | see general notes* |
| H82001_a01 | TrAa01MblScI | HI $\rightarrow$ $H^+$(aq) + $I^-$(aq) | $k_{\rm mt}(\rm HI) \cdot lwc$ | see general notes* |
| H82002_a01 | TrAa01ScI | $HIO_3$ $\rightarrow$ $IO_3^-$(aq) + $H^+$(aq) | $k_{\rm mt}(\rm HIO_3) \cdot lwc$ | see general notes* |
| H83000_a01 | TrAa01IN | $INO_2$ $\rightarrow$ HOI(aq) + HONO(aq) | k_exf(01,ind_INO2) | see general notes* |
| H83001_a01 | TrAa01MblIN | $INO_3$ $\rightarrow$ HOI(aq) + $HNO_3$(aq) | k_exf(01,ind_INO3) | see general notes* |
| H86000f_a01 | TrAa01MblScClI | ICl $\rightarrow$ ICl(aq) | k_exf(01,ind_ICl) | see general notes* |
| H86000b_a01 | TrAa01MblScClI | ICl(aq) $\rightarrow$ ICl | k_exb(01,ind_ICl) | see general notes* |
| H87000f_a01 | TrAa01MblScBrI | IBr $\rightarrow$ IBr(aq) | k_exf(01,ind_IBr) | see general notes* |
| H87000b_a01 | TrAa01MblScBrI | IBr(aq) $\rightarrow$ IBr | k_exb(01,ind_IBr) | see general notes* |
| H91000f_a01 | TrAa01MblScScmS | $SO_2$ $\rightarrow$ $SO_2$(aq) | k_exf(01,ind_SO2) | see general notes* |
| H91000b_a01 | TrAa01MblScScmS | $SO_2$(aq) $\rightarrow$ $SO_2$ | k_exb(01,ind_SO2) | see general notes* |
| H92000_a01 | TrAa01MblScScmS | $H_2SO_4$ $\rightarrow$ $H_2SO_4$(aq) | xnom7sulf*k_exf(01,ind_H2SO4) | see general notes* |
| H94000f_a01 | TrAa01CS | DMSO $\rightarrow$ DMSO(aq) | k_exf(01,ind_DMSO) | see general notes* |
| H94000b_a01 | TrAa01CS | DMSO(aq) $\rightarrow$ DMSO | k_exb(01,ind_DMSO) | see general notes* |
| H94001_a01 | TrAa01MblS | $CH_3SO_3H$ $\rightarrow$ $CH_3SO_3^-$(aq) + $H^+$(aq) | k_exf(01,ind_CH3SO3H) | see general notes* |
| H94002f_a01 | TrAa01CS | DMS $\rightarrow$ DMS(aq) | k_exf(01,ind_DMS) | see general notes* |
| H94002b_a01 | TrAa01CS | DMS(aq) $\rightarrow$ DMS | k_exb(01,ind_DMS) | see general notes* |
| H100000f_a01 | TrAa01Hg | Hg $\rightarrow$ Hg(aq) | k_exf(01,ind_Hg) | see general notes* |
| H100000b_a01 | TrAa01Hg | Hg(aq) $\rightarrow$ Hg | k_exb(01,ind_Hg) | see general notes* |
| H100100f_a01 | TrAa01Hg | HgO $\rightarrow$ HgO(aq) | k_exf(01,ind_HgO) | see general notes* |
| H100100b_a01 | TrAa01Hg | HgO(aq) $\rightarrow$ HgO | k_exb(01,ind_HgO) | see general notes* |
| H100600f_a01 | TrAa01ClHg | $HgCl_2$ $\rightarrow$ $HgCl_2$(aq) | k_exf(01,ind_HgCl2) | see general notes* |
| H100600b_a01 | TrAa01ClHg | $HgCl_2$(aq) $\rightarrow$ $HgCl_2$ | k_exb(01,ind_HgCl2) | see general notes* |
| H100700f_a01 | TrAa01BrHg | $HgBr_2$ $\rightarrow$ $HgBr_2$(aq) | k_exf(01,ind_HgBr2) | see general notes* |
| H100700b_a01 | TrAa01BrHg | $HgBr_2$(aq) $\rightarrow$ $HgBr_2$ | k_exb(01,ind_HgBr2) | see general notes* |
| H100701f_a01 | TrAa01BrClHg | ClHgBr $\rightarrow$ ClHgBr(aq) | k_exf(01,ind_ClHgBr) | see general notes* |
| H100701b_a01 | TrAa01BrClHg | ClHgBr(aq) $\rightarrow$ ClHgBr | k_exb(01,ind_ClHgBr) | see general notes* |
| H100702f_a01 | TrAa01BrHg | BrHgOBr $\rightarrow$ BrHgOBr(aq) | k_exf(01,ind_BrHgOBr) | see general notes* |
| H100702b_a01 | TrAa01BrHg | BrHgOBr(aq) $\rightarrow$ BrHgOBr | k_exb(01,ind_BrHgOBr) | see general notes* |
| H100703f_a01 | TrAa01BrClHg | ClHgOBr $\rightarrow$ ClHgOBr(aq) | k_exf(01,ind_ClHgOBr) | see general notes* |
| H100703b_a01 | TrAa01BrClHg | ClHgOBr(aq) $\rightarrow$ ClHgOBr | k_exb(01,ind_ClHgOBr) | see general notes* |

## General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry's law constants from chemprop (see `chemprop.pdf`).

For uptake of X (X = $N_2O_5$, $ClNO_3$, or $BrNO_3$) and subsequent reaction with $H_2O$, $Cl^-$, and $Br^-$ in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\mathrm{exf}}(\mathrm{X}) = \frac{k_{\mathrm{mt}}(\mathrm{X}) \times \mathrm{LWC}}{[\mathrm{H_2O}] + 5 \times 10^2[\mathrm{Cl^-}] + 3 \times 10^5[\mathrm{Br^-}]}$$

Here, $k_{\mathrm{mt}}$ = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by $k_{\mathrm{mt}}$. The factors only affect the branching between hydrolysis and the halide reactions. The factor $5\times10^2$ was chosen such that the chloride reaction dominates over hydrolysis at about $[Cl^-] > 0.1$ M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[H_2O]/[Cl^-]$ is less than $5\times10^2$. The ratio $5\times10^2/3\times10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of $N_2O_5$. Here, they are also used for $ClNO_3$ and $BrNO_3$.

Table 4: Heterogeneous reactions

| # | labels | reaction | rate coefficient | reference |
|---|---|---|---|---|
| HET300 | StHetN | $N_2O_5 + H_2O \rightarrow 2\ HNO_3$ | khet_St(ihs_N2O5_H2O) | see general notes* |
| HET301 | TrHetN | $N_2O_5 \rightarrow 2\ NO_3^-(cs) + 2\ H^+(cs)$ | khet_Tr(iht_N2O5) | see general notes* |
| HET610 | StHetCl | $HOCl + HCl \rightarrow Cl_2 + H_2O$ | khet_St(ihs_HOCl_HCl) | see general notes* |
| HET620 | StHetClN | $ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$ | khet_St(ihs_ClNO3_HCl) | see general notes* |
| HET621 | StHetClN | $ClNO_3 + H_2O \rightarrow HOCl + HNO_3$ | khet_St(ihs_ClNO3_H2O) | see general notes* |
| HET622 | StHetClN | $N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$ | khet_St(ihs_N2O5_HCl) | see general notes* |
| HET710 | StHetBr | $HOBr + HBr \rightarrow Br_2 + H_2O$ | khet_St(ihs_HOBr_HBr) | see general notes* |
| HET720 | StHetBrN | $BrNO_3 + H_2O \rightarrow HOBr + HNO_3$ | khet_St(ihs_BrNO3_H2O) | see general notes* |
| HET740 | StHetBrClN | $ClNO_3 + HBr \rightarrow BrCl + HNO_3$ | khet_St(ihs_ClNO3_HBr) | see general notes* |
| HET741 | StHetBrClN | $BrNO_3 + HCl \rightarrow BrCl + HNO_3$ | khet_St(ihs_BrNO3_HCl) | see general notes* |
| HET742 | StHetBrCl | $HOCl + HBr \rightarrow BrCl + H_2O$ | khet_St(ihs_HOCl_HBr) | see general notes* |
| HET743 | StHetBrCl | $HOBr + HCl \rightarrow BrCl + H_2O$ | khet_St(ihs_HOBr_HCl) | see general notes* |
| HET1001 | StTrHetHg | $Hg \rightarrow Hg(cs)$ | khet_Tr(iht_Hg) + khet_St(ihs_Hg) | see general notes* |
| HET1002 | StTrHetHg | $HgO \rightarrow Hg(cs)$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1003 | StTrHetClHg | $HgCl \rightarrow Hg(cs) + LCHLORINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1004 | StTrHetClHg | $HgCl_2 \rightarrow Hg(cs) + 2\ LCHLORINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1005 | StTrHetBrHg | $HgBr \rightarrow Hg(cs) + LBROMINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1006 | StTrHetBrHg | $HgBr_2 \rightarrow Hg(cs) + 2\ LBROMINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1007 | StTrHetBrClHg | $ClHgBr \rightarrow Hg(cs) + LCHLORINE + LBROMINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1008 | StTrHetBrHg | $BrHgOBr \rightarrow Hg(cs) + 2\ LBROMINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |
| HET1009 | StTrHetBrClHg | $ClHgOBr \rightarrow Hg(cs) + LCHLORINE + LBROMINE$ | khet_Tr(iht_RGM) + khet_St(ihs_RGM) | see general notes* |

# General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA_KHET) and then supplied to the MECCA chemistry (see www.messy-interface.org for details)

Table 5: Acid-base and other equilibria

| # | labels | reaction | $K_0[M^{m-n}]$ | $-\Delta H/R[K]$ | reference |
|---|---|---|---|---|---|
| EQ2100_a01 | TrAa01Sc | $HO_2 \rightleftharpoons O_2^- + H^+$ | 1.6E-5 | | Weinstein-Lloyd and Schwartz (1991) |
| EQ2101_a01 | TrAa01MblScScm | $H_2O \rightleftharpoons H^+ + OH^-$ | 1.0E-16 | -6716 | Chameides (1984) |
| EQ2102_a01 | TrAa01Sc | $HO_3 \rightleftharpoons O_3^- + H^+$ | 4.4E-9 | | Staehelin et al. (1984) |
| EQ3200_a01 | TrAa01MblScScmN | $NH_4^+ \rightleftharpoons H^+ + NH_3$ | 5.88E-10 | -2391 | Chameides (1984) |
| EQ3201_a01 | TrAa01ScN | $HONO \rightleftharpoons H^+ + NO_2^-$ | 5.1E-4 | -1260 | Schwartz and White (1981) |
| EQ3202_a01 | TrAa01MblScScmN | $HNO_3 \rightleftharpoons H^+ + NO_3^-$ | 15 | 8700 | Davis and de Bruin (1964) |
| EQ3203_a01 | TrAa01ScN | $HNO_4 \rightleftharpoons NO_4^- + H^+$ | 1.E-5 | | Warneck (1999) |
| EQ4100_a01 | TrAa01MblScScm | $CO_2 \rightleftharpoons H^+ + HCO_3^-$ | 4.3E-7 | -913 | Chameides (1984)* |
| EQ4101_a01 | TrAa01ScScm | $HCOOH \rightleftharpoons H^+ + HCOO^-$ | 1.8E-4 | | Weast (1980) |
| EQ4150_a01 | TrAa01Sc | $HCHO \rightleftharpoons HOCH_2OH$ | 4.11E-3 | -3769 | see note* |
| EQ4151_a01 | TrAa01Sc | $HCO_3 \rightleftharpoons HCOHOHO_2$ | 1.08E1 | -2936 | see note* |
| EQ4201_a01 | TrAa01ScC | $CH_3C(O)OOH \rightleftharpoons CH_3COOO^- + H^+$ | 6.3E-9 | | Schuchmann and von Sonntag (1988) |
| EQ4202_a01 | TrAa01ScC | $HOCH_2CO_3H \rightleftharpoons CH_2OHCO_2O^- + H^+$ | 6.3E-9 | | Schuchmann and von Sonntag (1988)* |
| EQ4203_a01 | TrAa01ScC | $HOOCCOOH \rightleftharpoons H^+ + HOOCCOO^-$ | 5.6E-2 | | Martell and Smith (1977) |
| EQ4204_a01 | TrAa01ScC | $HOOCCOO^- \rightleftharpoons H^+ + C_2O_4^{2-}$ | 5.4E-5 | | Martell and Smith (1977) |
| EQ4205_a01 | TrAa01ScC | $HOOCH2CO2H \rightleftharpoons H^+ + CH_2OOHCO_2^-$ | 1.754E-5 | | Fisher and Barnes (1972)* |
| EQ4206_a01 | TrAa01ScC | $CH_2OOCOOH \rightleftharpoons H^+ + CH_2OOCO_2^-$ | 1.754E-5 | | Fisher and Barnes (1972)* |
| EQ4207_a01 | TrAa01ScC | $CHOOHOOCOOH \rightleftharpoons H^+ + CHOOHOOCO_2^-$ | 1.754E-5 | | Fisher and Barnes (1972)* |
| EQ4208_a01 | TrAa01ScC | $HOCH_2CO_2H \rightleftharpoons H^+ + CH_2OHCO_2^-$ | 1.5E-4 | | Rumble (2020) |
| EQ4209_a01 | TrAa01ScC | $CHOHOOCOOH \rightleftharpoons H^+ + CHOHOOCOO_2^-$ | 1.5E-4 | | Rumble (2020)* |
| EQ4210_a01 | TrAa01ScC | $CHOCOOH \rightleftharpoons H^+ + CHOCOO^-$ | 1.754E-5 | | Fisher and Barnes (1972) |
| EQ4211_a01 | TrAa01ScC | $COOHCO_3 \rightleftharpoons H^+ + CO_2^-CO_3$ | 1.754E-5 | | Fisher and Barnes (1972) |
| EQ4250_a01 | TrAa01ScC | $CH_3CHO \rightleftharpoons CH_3CHOHOH$ | 1.22 | | Tur'yan (2000) |
| EQ4251_a01 | TrAa01ScC | $CHOHOOCHO \rightleftharpoons CHOHOOCHOHOH$ | 1.57E1 | | see note* |
| EQ4252_a01 | TrAa01ScC | $CH_2OHCHO \rightleftharpoons CH_2OHCHOHOH$ | 1.56E1 | | Doussin and Monod (2013) |
| EQ4253_a01 | TrAa01ScC | $GLYOX \rightleftharpoons CHOCHOHOH$ | 3.5E2 | | Ervens and Volkamer (2010) |
| EQ4254_a01 | TrAa01ScC | $CHOCHOHOH \rightleftharpoons CHOHOHCHOHOH$ | 2.0E2 | | Ervens and Volkamer (2010) |
| EQ4255_a01 | TrAa01ScC | $CHOCOOH \rightleftharpoons CHOOHOHCOOH$ | 1.1E3 | | Doussin and Monod (2013) |
| EQ4256_a01 | TrAa01ScC | $CHOCOO^- \rightleftharpoons CHOHOHCO_2^-$ | 6.6E1 | | Doussin and Monod (2013) |
| EQ4257_a01 | TrAa01ScC | $CO_2^-CO_3 \rightleftharpoons CO2^-COHOHO_2$ | 6.6E1 | | see note* |
| EQ4258_a01 | TrAa01ScC | $CH_2OOHCHO \rightleftharpoons HOOCH_2CHOHOH$ | 1.56E1 | | see note* |
| EQ4300_a01 | TrAa01ScScmC | $CH_3COCOOH \rightleftharpoons H^+ + CH_3COCO2^-$ | 4.1E-3 | | Rumble (2020) |
| EQ4350_a01 | TrAa01ScC | $CH_3C(O)CHO \rightleftharpoons CH_3COCHOHOH$ | 1.98E3 | | Doussin and Monod (2013) |

Table 5: Acid-base and other equilibria

| # | labels | reaction | $K_0[M^{m-n}]$ | $-\Delta H/R[K]$ | reference |
|---|---|---|---|---|---|
| EQ6000_a01 | TrAa01Cl | $Cl_2^- \rightleftharpoons Cl + Cl^-$ | 7.3E-6 | | Yu (2004) |
| EQ6200_a01 | TrAa01MblScScmCl | $HCl \rightleftharpoons H^+ + Cl^-$ | 1.7E6 | 6896 | Marsh and McElroy (1985) |
| EQ6201_a01 | TrAa01ScCl | $HOCl \rightleftharpoons H^+ + ClO^-$ | 3.2E-8 | | Lax (1969) |
| EQ7000_a01 | TrAa01Br | $Br_2^- \rightleftharpoons Br + Br^-$ | 2.54E-6 | -2256 | Liu et al. (2002) |
| EQ7200_a01 | TrAa01MblScScmBr | $HBr \rightleftharpoons H^+ + Br^-$ | 1.0E9 | | Lax (1969) |
| EQ7201_a01 | TrAa01ScBr | $HOBr \rightleftharpoons H^+ + BrO^-$ | 2.3E-9 | -3091 | Kelley and Tartar (1956)* |
| EQ7600_a01 | TrAa01MblBrCl | $BrCl + Cl^- \rightleftharpoons BrCl_2^-$ | 3.8 | 1191 | Wang et al. (1994) |
| EQ7601_a01 | TrAa01MblBrCl | $BrCl + Br^- \rightleftharpoons Br_2Cl^-$ | 1.8E4 | 7457 | Wang et al. (1994) |
| EQ7602_a01 | TrAa01MblBrCl | $Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$ | 1.3 | 0 | Wang et al. (1994) |
| EQ7603_a01 | TrAa01MblBrCl | $Br^- + Cl_2 \rightleftharpoons BrCl_2^-$ | 4.2E6 | 14072 | Wang et al. (1994) |
| EQ8600_a01 | TrAa01MblScClI | $ICl + Cl^- \rightleftharpoons ICl_2^-$ | 7.7E1 | | Wang et al. (1989) |
| EQ8700_a01 | TrAa01MblScBrI | $IBr + Br^- \rightleftharpoons IBr_2^-$ | 2.9E2 | | Troy and Margerum (1991) |
| EQ8701_a01 | TrAa01MblScBrClI | $ICl + Br^- \rightleftharpoons IBr + Cl^-$ | 3.3E2 | | see note* |
| EQ9200_a01 | TrAa01MblScScmS | $SO_2 \rightleftharpoons H^+ + HSO_3^-$ | 1.7E-2 | 2090 | Chameides (1984) |
| EQ9201_a01 | TrAa01MblScScmS | $HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$ | 6.0E-8 | 1120 | Chameides (1984) |
| EQ9202_a01 | TrAa01MblScScmS | $HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$ | 1.2E-2 | 2720 | Seinfeld and Pandis (1998) |
| EQ9203_a01 | TrAa01MblScScmS | $H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$ | 1.0E3 | | Seinfeld and Pandis (1998) |
| EQ10200_a01 | TrAa01Hg | $Hg^{2+} + OH^- \rightleftharpoons HgOH^+$ | 4.0E10 | | Ammann and Pöschl (2007) |
| EQ10201_a01 | TrAa01Hg | $HgOH^+ + OH^- \rightleftharpoons Hg(OH)_2$ | 1.58E11 | | Ammann and Pöschl (2007) |
| EQ10600_a01 | TrAa01ClHg | $Hg^{2+} + Cl^- \rightleftharpoons HgCl^+$ | 5.8E6 | | Ammann and Pöschl (2007) |
| EQ10601_a01 | TrAa01ClHg | $HgCl^+ + Cl^- \rightleftharpoons HgCl_2$ | 2.5E6 | | Ammann and Pöschl (2007) |
| EQ10602_a01 | TrAa01ClHg | $HgOH^+ + Cl^- \rightleftharpoons Hg(OH)Cl$ | 2.69E7 | | Ammann and Pöschl (2007) |
| EQ10700_a01 | TrAa01BrHg | $Hg^{2+} + Br^- \rightleftharpoons HgBr^+$ | 1.1E9 | | Raofie and Ariya (2004) |
| EQ10701_a01 | TrAa01BrHg | $HgBr^+ + Br^- \rightleftharpoons HgBr_2$ | 2.5E8 | | Raofie and Ariya (2004) |
| EQ10800_a01 | TrAa01HgS | $Hg^{2+} + SO_3^{2-} \rightleftharpoons HgSO_3$ | 2.E13 | | van Loon et al. (2001) |
| EQ10801_a01 | TrAa01HgS | $HgSO_3 + SO_3^{2-} \rightleftharpoons Hg(SO_3)_2^{2-}$ | 1.E10 | | van Loon et al. (2001) |
| EQ11200_a01 | TrAa01Fe | $Fe^{3+} \rightleftharpoons FeOH^{2+} + H^+$ | 2.34E-3 | | de Laat and Le (2006)* |
| EQ11201_a01 | TrAa01Fe | $FeOH^{2+} \rightleftharpoons Fe(OH)_2^+ + H^+$ | 2E-4 | | de Laat and Le (2006)* |
| EQ11202_a01 | TrAa01Fe | $Fe^{3+} + H_2O_2 \rightleftharpoons FeHO_2^{2+} + H^+$ | 3.1E-3 | | de Laat and Le (2006) |
| EQ11203_a01 | TrAa01Fe | $FeOH^{2+} + H_2O_2 \rightleftharpoons Fe(OH)(HO_2)^+ + H^+$ | 2E-4 | | de Laat and Le (2006) |
| EQ11600_a01 | TrAa01ClFe | $Fe^{3+} + Cl^- \rightleftharpoons FeCl^{2+}$ | 6.61 | | de Laat and Le (2006)* |
| EQ11601_a01 | TrAa01ClFe | $FeCl^{2+} + Cl^- \rightleftharpoons FeCl_2^+$ | 1.6 | | de Laat and Le (2006)* |
| EQ11800_a01 | TrAa01FeS | $Fe^{3+} + SO_4^{2-} \rightleftharpoons FeSO_4^+$ | 120 | | Brand and van Eldik (1995)* |
| EQ11801_a01 | TrAa01FeS | $FeOH^{2+} + HSO_3^- \rightleftharpoons FeSO_3^+$ | 8.25E2 | | Warneck (2018)* |

Table 5: Acid-base and other equilibria

| # | labels | reaction | $K_0[M^{m-n}]$ | $-\Delta H/R[K]$ | reference |
|---|---|---|---|---|---|
| EQ11802_a01 | TrAa01FeS | $Fe^{2+} + SO_3^- \rightleftharpoons FeSO_3^+$ | 1.6E7 | | Warneck (2018) |

## Specific notes

EQ4100_a01: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

EQ4150_a01: Hydration from Winkelman et al. (2000) and dehydration from Winkelman et al. (2002). Bell and Evans (1966) found that acid catalysis is negligible.

EQ4151_a01: Assumed to be the same as for HCHO.

EQ4202_a01: Same as for CH3CO3H.

EQ4205_a01: Same as for CH3CO2H.

EQ4206_a01: Same as for CH3CO2H.

EQ4207_a01: Same as for CH3CO2H.

EQ4209_a01: Same as HOCH2CO2H.

EQ4251_a01: Calculated as $K_{\mathrm{eq}}$ * $k$(dehydration) where dehydration is assumed to be the same as for acetaldehyde.

EQ4257_a01: Assumed to be equal to CHOCO2m.

EQ4258_a01: Same as for $HOCH_2CHO$.

EQ7201_a01: For $pK_a$(HOBr), see also Keller-Rudek et al. (1992).

EQ8701_a01: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):

$$\begin{array}{ccccccc} \mathrm{ICl} & + & \mathrm{Br^-} & \rightleftharpoons & \mathrm{IBr} & + & \mathrm{Cl^-} \\ -17.1 & & -103.96 & = & -4.2 & & -131.228 \end{array}$$

$$\frac{\Delta G}{[\mathrm{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\mathrm{IBr}] \times [\mathrm{Cl^-}]}{[\mathrm{ICl}] \times [\mathrm{Br^-}]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[Cl^-]/[Br^-]$ ratio equals 330.

EQ11200_a01: See also $K$ values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11201_a01: Equilibrium calculated from $K_1$ and $K_2$ in Tab. 1 of de Laat and Le (2006). $k$ for back reaction assumed. See also $K$ values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11600_a01: See also $K$ values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11601_a01: Equilibrium calculated from $K_{29}$ and $K_{30}$ in Tab. 2 of de Laat and Le (2006). $k$ for forward reaction assumed. See also $K$ values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11800_a01: Equilibrium at $I = 1$ M. $k$ for back reaction assumed.

EQ11801_a01: Rate of equilibration assumed.

Table 6: Aqueous phase reactions

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A10000_a01 | TrAa01Sc | $O_3 + O_2^- \rightarrow O_3^- + O_2$ | 1.50E9 | | Staehelin et al. (1984) |
| A21000_a01 | TrAa01Sc | $OH + O_2^- \rightarrow OH^-$ | 1.0E10 | | Sehested et al. (1968) |
| A21001_a01 | TrAa01Sc | $OH + OH \rightarrow H_2O_2$ | 5.5E9 | | Buxton et al. (1988) |
| A21002_a01 | TrAa01Sc | $HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$ | 1.0E8 | -900 | Christensen and Sehested (1988) |
| A21003_a01 | TrAa01Sc | $HO_2 + OH \rightarrow H_2O$ | 7.1E9 | | Sehested et al. (1968) |
| A21004_a01 | TrAa01Sc | $HO_2 + HO_2 \rightarrow H_2O_2$ | 9.7E5 | -2500 | Christensen and Sehested (1988) |
| A21005_a01 | TrAa01Sc | $H_2O_2 + OH \rightarrow HO_2$ | 2.7E7 | -1684 | Christensen et al. (1982) |
| A21006_a01 | TrAa01Sc | $O_3 + OH \rightarrow HO_4$ | 1.10E8 | | Staehelin et al. (1984) |
| A21007_a01 | TrAa01Sc | $O_3 + OH^- \rightarrow HO_2 + O_2^-$ | 7.00E1 | | Staehelin et al. (1984) |
| A21008_a01 | TrAa01Sc | $HO_3 \rightarrow OH + O_2$ | 1.10E5 | | Staehelin et al. (1984) |
| A21009_a01 | TrAa01Sc | $HO_4 \rightarrow HO_2 + O_2$ | 2.80E4 | | Staehelin et al. (1984) |
| A21010_a01 | TrAa01Sc | $HO_4 + HO_4 \rightarrow H_2O_2 + 2\ O_3$ | 5.00E9 | | Staehelin et al. (1984) |
| A21011_a01 | TrAa01Sc | $HO_4 + HO_3 \rightarrow H_2O_2 + O_3 + O_2$ | 5.00E9 | | Staehelin et al. (1984) |
| A31000_a01 | TrAa01ScN | $NO_2^- + O_3 \rightarrow NO_3^-$ | 5.0E5 | -6950 | Damschen and Martin (1983) |
| A31001_a01 | TrAa01ScN | $NO_2 + NO_2 \rightarrow HNO_3 + HONO$ | 1.0E8 | | Lee and Schwartz (1981) |
| A31002_a01 | TrAa01ScN | $NO_4^- \rightarrow NO_2^-$ | 8.0E1 | | Warneck (1999) |
| A32000_a01 | TrAa01ScN | $NO_2 + HO_2 \rightarrow HNO_4$ | 1.8E9 | | Warneck (1999) |
| A32001_a01 | TrAa01ScN | $NO_2^- + OH \rightarrow NO_2 + OH^-$ | 1.0E10 | | Wingenter et al. (1999) |
| A32002_a01 | TrAa01ScN | $NO_3 + OH^- \rightarrow NO_3^- + OH$ | 8.2E7 | -2700 | Exner et al. (1992) |
| A32003_a01 | TrAa01ScN | $HONO + OH \rightarrow NO_2$ | 1.0E10 | | Barker et al. (1970) |
| A32004_a01 | TrAa01ScN | $HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$ | 4.6E3 | -6800 | Damschen and Martin (1983) |
| A41000_a01 | TrAa01Sc | $CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$ | 6.5E8 | | Ross et al. (1992) |
| A41001_a01 | TrAa01Sc | $CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$ | 4.3E5 | | Ross et al. (1992) |
| A41002_a01 | TrAa01Sc | $HCOO^- + CO_3^- \rightarrow 2\ HCO_3^- + HO_2$ | 1.5E5 | | Ross et al. (1992) |
| A41003_a01 | TrAa01Sc | $HCOO^- + OH \rightarrow O_2^- + H_2O + CO_2$ | 3.1E9 | -1240 | Chin and Wine (1994) |
| A41004_a01 | TrAa01ScN | $HCOO^- + NO_3 \rightarrow NO_3^- + H^+ + O_2^- + CO_2$ | 5.119E+07 | -2200 | Exner et al. (1994) |
| A41005_a01 | TrAa01Sc | $HCOO^- + O_3 \rightarrow OH + O_2^- + CO_2$ | 1.00E2 | | Hoigné and Bader (1983) |
| A41006_a01 | TrAa01Sc | $HCO_3^- + OH \rightarrow CO_3^-$ | 8.5E6 | | Ross et al. (1992) |
| A41007_a01 | TrAa01Sc | $HCHO + OH \rightarrow HCOOH + HO_2$ | 7.7E8 | -1020 | Chin and Wine (1994) |
| A41008_a01 | TrAa01Sc | $HCOOH + OH \rightarrow HO_2 + CO_2$ | 1.1E8 | -991 | Chin and Wine (1994) |
| A41009_a01 | TrAa01ScN | $HCOOH + NO_3 \rightarrow NO_3^- + H^+ + HO_2 + CO_2$ | 3.8E5 | -3400 | Exner et al. (1994) |
| A41010_a01 | TrAa01Sc | $CH_3OO + HO_2 \rightarrow CH_3OOH$ | 4.3E5 | | Jacob (1986) |
| A41011_a01 | TrAa01Sc | $CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$ | 5.0E7 | | Jacob (1986) |
| A41012a_a01 | TrAa01Sc | $CH_3OO + CH_3OO \rightarrow 2\ HCHO + H_2O_2$ | 0.20 × 2.145E+08 | -2139 | Herrmann et al. (1999b) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A41012b_a01 | TrAa01Sc | $CH_3OO + CH_3OO \rightarrow 2\ HOCH_2O_2$ | 0.80 × 2.145E+08 | -2139 | Herrmann et al. (1999b) |
| A41013a_a01 | TrAa01Sc | $CH_3OH + OH \rightarrow HOCH_2O_2 + H_2O$ | 0.93 × 9.70E8 | -600 | Elliot and McCracken (1989)* |
| A41013b_a01 | TrAa01Sc | $CH_3OH + OH \rightarrow HCHO + HO_2 + H_2O$ | 0.07 × 9.70E8 | -600 | Elliot and McCracken (1989) |
| A41014_a01 | TrAa01ScN | $CH_3OH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$ | 5.40E5 | -4300 | Herrmann and Zellner (1998) |
| A41015_a01 | TrAa01Sc | $CH_3OH + CO_3^- \rightarrow HOCH_2O_2 + HCO_3^-$ | 5.431E+03 | -3100 | Clifton and Huie (1993) |
| A41016a_a01 | TrAa01Sc | $CH_3OOH + OH \rightarrow CH_3OO + H_2O$ | 0.25 × 6.30E8 | | Monod et al. (2007)* |
| A41016b_a01 | TrAa01Sc | $CH_3OOH + OH \rightarrow HCHO + OH + H_2O$ | 0.75 × 6.30E8 | | Monod et al. (2007)* |
| A41017a_a01 | TrAa01ScN | $CH_3OOH + NO_3 \rightarrow CH_3OO + NO_3^- + H^+$ | 0.25 × 4.90E6 | -2000 | see note* |
| A41017b_a01 | TrAa01ScN | $CH_3OOH + NO_3 \rightarrow HCHO + HO_2 + NO_3^- + H^+$ | 0.75 × 4.90E6 | -2000 | see note* |
| A41018a_a01 | TrAa01Sc | $CH_3OOH + CO_3^- \rightarrow CH_3OO + HCO_3^-$ | 0.25 × 4.30E5 | | see note* |
| A41018b_a01 | TrAa01Sc | $CH_3OOH + CO_3^- \rightarrow HCHO + HO_2 + HCO_3^-$ | 0.75 × 4.30E5 | | see note* |
| A41019a_a01 | TrAa01Sc | $HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$ | 0.25 × 6.30E8 | | see note* |
| A41019b_a01 | TrAa01Sc | $HOCH_2OOH + OH \rightarrow CHOOOH + HO_2 + H_2O$ | 0.75 × 6.30E8 | | see note* |
| A41020a_a01 | TrAa01ScN | $HOCH_2OOH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$ | 0.25 × 4.90E6 | -2000 | see note* |
| A41020b_a01 | TrAa01ScN | $HOCH_2OOH + NO_3 \rightarrow CHOOOH + HO_2 + NO_3^- + H^+$ | 0.75 × 4.90E6 | -2000 | see note* |
| A41021_a01 | TrAa01Sc | $HOCH_2O_2 \rightarrow HCHO + HO_2$ | 1.00E1 | | see note* |
| A41022_a01 | TrAa01Sc | $HOCH_2O_2 + HO_2 \rightarrow HOCH_2OOH + O_2$ | 9.7E5 | -2500 | see note* |
| A41023_a01 | TrAa01Sc | $HOCH_2O_2 + O_2^- \rightarrow HOCH_2OOH + O_2 + OH^-$ | 1.0E8 | -900 | see note* |
| A41024_a01 | TrAa01Sc | $HOCH_2O_2 + HOCH_2O_2 \rightarrow 2\ HCOOH + H_2O_2$ | 7.367E+08 | -1395 | Huie and Clifton (1993) |
| A41025_a01 | TrAa01Sc | $HCOOH + H_2O_2 + H^+ \rightarrow CHOOOH + H_2O + H^+$ | 3.080E-04 | -5235 | De Filippis et al. (2009) |
| A41026a_a01 | TrAa01Sc | $CHOOOH + H^+ \rightarrow HCOOH + H_2O_2 + H^+$ | 3.790E-04 | -5235 | De Filippis et al. (2009) |
| A41026b_a01 | TrAa01Sc | $CHOOOH + H^+ \rightarrow CO_2 + H_2O + H^+$ | 1.219E-03 | -8735 | De Filippis et al. (2009) |
| A41027_a01 | TrAa01Sc | $HOCH_2OH + OH \rightarrow HCOHOHO_2 + H_2O$ | 7.70E8 | -1000 | Chin and Wine (1994) |
| A41028_a01 | TrAa01Sc | $HOCH_2OH + CO_3^- \rightarrow HCO_3^- + HCOHOHO_2$ | 1.30E4 | | Zellner et al. (1996) |
| A41029_a01 | TrAa01ScN | $HOCH_2OH + NO_3 \rightarrow NO_3^- + H^+ + HCOHOHO_2$ | 1.003E+06 | -4500 | Exner et al. (1993) |
| A41030_a01 | TrAa01Sc | $HCOHOHO_2 \rightarrow HCOOH + HO_2$ | 1.00E6 | | see note* |
| A42000a_a01 | TrAa01ScC | $CH_3CH_2OH + OH \rightarrow CH_3CHO + HO_2 + H_2O$ | 0.90 × 2.002E+09 | -830 | Monod et al. (2005)* |
| A42000b_a01 | TrAa01ScC | $CH_3CH_2OH + OH \rightarrow CH_2OHCH_2OO + H_2O$ | 0.10 × 2.002E+09 | -830 | Monod et al. (2005) |
| A42001a_a01 | TrAa01ScCN | $CH_3CH_2OH + NO_3 \rightarrow CH_3CHO + HO_2 + NO_3^- + H^+$ | 0.90 × 2.184E+06 | -3300 | Herrmann and Zellner (1998)* |
| A42001b_a01 | TrAa01ScCN | $CH_3CH_2OH + NO_3 \rightarrow CH_2OHCH_2OO + NO_3^- + H^+$ | 0.10 × 2.184E+06 | -3300 | Herrmann and Zellner (1998) |
| A42002a_a01 | TrAa01ScC | $CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow CH_2OHCHO + CH_2OHCHO + H_2O_2$ | 0.50 × 1.00E8 | | Piesiak et al. (1984) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A42002b_a01 | TrAa01ScC | $CH_2OHCH_2OO$ + $CH_2OHCH_2OO$ → $CH_2OHCHO$ + ETHGLY | 0.33 × 1.00E8 | | Piesiak et al. (1984) |
| A42002c_a01 | TrAa01ScC | $CH_2OHCH_2OO$ + $CH_2OHCH_2OO$ → 2 $HOCH_2O_2$ + 2 HCHO | 0.17 × 1.00E8 | | Piesiak et al. (1984) |
| A42003_a01 | TrAa01ScC | $CH_2OHCH_2OO$ + $O_2^-$ → HYETHO2H + $OH^-$ | 1.0E8 | -900 | see note* |
| A42004_a01 | TrAa01ScC | $CH_2OHCH_2OO$ + $HO_2$ → HYETHO2H | 9.7E5 | -2500 | see note* |
| A42005_a01 | TrAa01ScC | HYETHO2H + OH → $CH_2OHCHO$ | 1.10E9 | | see note* |
| A42006_a01 | TrAa01ScC | ETHGLY + OH → $CH_2OHCHO$ + $HO_2$ + $H_2O$ | 1.657E+09 | -1191 | Hoffmann et al. (2009)* |
| A42007_a01 | TrAa01ScCN | ETHGLY + $NO_3$ → $CH_2OHCHO$ + $HO_2$ + $NO_3^-$ + $H^+$ | 5.856E+06 | -2117 | Hoffmann et al. (2009)* |
| A42008_a01 | TrAa01ScC | $CH_3CHO$ + OH → $CH_3COOO$ + $H_2O$ | 3.60E9 | | Schuchmann and von Sonntag (1988) |
| A42009_a01 | TrAa01ScCN | $CH_3CHO$ + $NO_3$ → $CH_3COOO$ + $NO_3^-$ + $H^+$ | 3.10E6 | | Rousse and George (2004) |
| A42010_a01 | TrAa01ScC | $CH_3COOO$ + $CH_3COOO$ → $CH_3OO$ + $CH_3OO$ + $CO_2$ + $CO_2$ | 1.891E+08 | 1563 | see note* |
| A42011_a01 | TrAa01ScC | $CH_3COOO$ + $O_2^-$ → $CH_3COOO^-$ + $O_2$ | 1.00E9 | | Schuchmann and von Sonntag (1988) |
| A42012_a01 | TrAa01ScC | $CH_3CHOHOH$ + OH → $CH_3COHOHOO$ + $H_2O$ | 1.20E9 | | Schuchmann and von Sonntag (1988) |
| A42013_a01 | TrAa01ScCN | $CH_3CHOHOH$ + $NO_3$ → $CH_3COHOHOO$ + $NO_3^-$ + $H^+$ | 1.10E6 | | Rousse and George (2004) |
| A42014_a01 | TrAa01ScC | $CH_3COHOHOO$ → $CH_3COOH$ + $HO_2$ | 1.00E6 | | see note* |
| A42015a_a01 | TrAa01ScC | $CH_2OHCHO$ + OH → $CH_2OHCO3$ + $H_2O$ | 0.77 × 1.40E9 | | Doussin and Monod (2013) |
| A42015b_a01 | TrAa01ScC | $CH_2OHCHO$ + OH → CHOHOOCHO + $H_2O$ | 0.23 × 1.40E9 | | Doussin and Monod (2013) |
| A42016a_a01 | TrAa01ScCN | $CH_2OHCHO$ + $NO_3$ → $CH_2OHCO3$ + $NO_3^-$ + $H^+$ | 0.77 × 3.10E6 | | see note* |
| A42016b_a01 | TrAa01ScCN | $CH_2OHCHO$ + $NO_3$ → CHOHOOCHO + $NO_3^-$ + $H^+$ | 0.23 × 3.10E6 | | see note* |
| A42017_a01 | TrAa01ScC | $CH_2OHCO3$ + $O_2^-$ → $CH_2OHCO_2O^-$ | 1.00E9 | | see note* |
| A42018_a01 | TrAa01ScC | $CH_2OHCOHOHO_2$ → $HOCH_2CO_2H$ + $HO_2$ | 1.00E6 | | see note* |
| A42019_a01 | TrAa01ScC | CHOHOOCHO → GLYOX + $HO_2$ | 1.90E2 | | see note* |
| A42020_a01 | TrAa01ScC | CHOHOOCHOHOH → CHOCHOHOH + $HO_2$ | 1.90E2 | | see note* |
| A42021a_a01 | TrAa01ScC | $CH_2OHCHOHOH$ + OH → $CH_2OHCOHOHO_2$ + $H_2O$ | 0.33 × 1.10E9 | | Doussin and Monod (2013) |
| A42021b_a01 | TrAa01ScC | $CH_2OHCHOHOH$ + OH → CHOHOOCHOHOH + $H_2O$ | 0.28 × 1.10E9 | | Doussin and Monod (2013) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A42021c_a01 | TrAa01ScC | $CH_2OHCHOHOH + OH \rightarrow HCOOH + HOCH_2O_2 + H_2O$ | 0.39 × 1.10E9 | | Doussin and Monod (2013) |
| A42022a_a01 | TrAa01ScCN | $CH_2OHCHOHOH + NO_3 \rightarrow CH_2OHCOHOHO_2 + NO_3^- + H^+$ | 0.33 × 1.10E6 | | see note* |
| A42022b_a01 | TrAa01ScCN | $CH_2OHCHOHOH + NO_3 \rightarrow CHOHOOCHOHOH + NO_3^- + H^+$ | 0.28 × 1.10E6 | | see note* |
| A42022c_a01 | TrAa01ScCN | $CH_2OHCHOHOH + NO_3 \rightarrow HCOOH + HOCH_2O_2 + NO_3^- + H^+$ | 0.39 × 1.10E6 | | see note* |
| A42023a_a01 | TrAa01ScC | $CHOHOHCHOHOH + OH \rightarrow CHOHOHCOHOHO_2 + H_2O$ | 0.27 × 1.114E+09 | -1516 | Buxton et al. (1997) |
| A42023b_a01 | TrAa01ScC | $CHOHOHCHOHOH + OH \rightarrow HCOOH + HCOHOHO_2 + HO_2 + H_2O$ | 0.73 × 1.114E+09 | -1516 | Buxton et al. (1997)* |
| A42024a_a01 | TrAa01ScCN | $CHOHOHCHOHOH + NO_3 \rightarrow CHOHOHCOHOHO_2 + NO_3^- + H^+$ | 0.27 × 1.00E6 | | see note* |
| A42024b_a01 | TrAa01ScCN | $CHOHOHCHOHOH + NO_3 \rightarrow HCOOH + HCOHOHO_2 + HO_2 + NO_3^- + H^+$ | 0.73 × 1.00E6 | | see note* |
| A42025_a01 | TrAa01ScC | $CHOHOHCOHOHO_2 \rightarrow CHOOHOHCOOH + HO_2$ | 0.77 × 1.00E6 | | see note* |
| A42026_a01 | TrAa01ScC | $CH_3COOH + OH \rightarrow CH_2OOCOOH + H_2O$ | 1.50E7 | -1330 | Chin and Wine (1994) |
| A42027_a01 | TrAa01ScCN | $CH_3COOH + NO_3 \rightarrow CH_2OOCOOH + NO_3^- + H^+$ | 1.429E+04 | -3800 | Exner et al. (1994) |
| A42028_a01 | TrAa01ScC | $CH_3COO^- + OH \rightarrow CH_2OOCO_2^- + H_2O$ | 1.00E8 | -1800 | Fisher and Hamill (1973) |
| A42029_a01 | TrAa01ScCN | $CH_3COO^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$ | 2.916E+06 | -3800 | Exner et al. (1994) |
| A42030a_a01 | TrAa01ScC | $C2H5OOH + OH \rightarrow C2H5OO + H_2O$ | 0.80 × 5.80E8 | | Monod et al. (2007) |
| A42030b_a01 | TrAa01ScC | $C2H5OOH + OH \rightarrow CH_3COOH + HO_2 + H_2O$ | 0.20 × 5.80E8 | | Monod et al. (2007)* |
| A42031a_a01 | TrAa01ScC | $C2H5OO + C2H5OO \rightarrow CH_3CHO + CH_3CHO + H_2O_2$ | 0.20 × 1.891E+08 | 1563 | Herrmann et al. (1999b) |
| A42031b_a01 | TrAa01ScC | $C2H5OO + C2H5OO \rightarrow 2\ CH_3CHO + 2\ HO_2$ | 0.80 × 1.891E+08 | 1563 | Herrmann et al. (1999b)* |
| A42032_a01 | TrAa01ScC | $C2H5OO + O_2^- \rightarrow C2H5OOH + OH^-$ | 1.0E8 | -900 | see note* |
| A42033_a01 | TrAa01ScC | $C2H5OO + HO_2 \rightarrow C2H5OOH$ | 9.7E5 | -2500 | see note* |
| A42034_a01 | TrAa01ScC | $CH_2OOCOOH + HO_2 \rightarrow HOOCH2CO2H$ | 9.7E5 | -2500 | see note* |
| A42035_a01 | TrAa01ScC | $CH_2OOCOOH + O_2^- + H^+ \rightarrow HOOCH2CO2H$ | 1.0E8 | -900 | see note* |
| A42036a_a01 | TrAa01ScC | $CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOCOOH + CHOCOOH + H_2O_2$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |
| A42036b_a01 | TrAa01ScC | $CH_2OOCOOH + CH_2OOCOOH \rightarrow 2\ HCHO + 2\ CO_2 + H_2O_2$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A42036c_a01 | TrAa01ScC | $CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOCOOH + HOCH_2CO_2H$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |
| A42036d_a01 | TrAa01ScC | $CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOHOOCOOH + CHOHOOCOOH$ | 0.10 × 7.50E7 | | Schuchmann et al. (1985) |
| A42037_a01 | TrAa01ScC | $CH_2OOCO_2^- + HO_2 \rightarrow CH_2OOHCO_2^- + O_2$ | 9.7E5 | -2500 | see note* |
| A42038_a01 | TrAa01ScC | $CH_2OOCO_2^- + O_2^- + H^+ \rightarrow CH_2OOHCO_2^-$ | 1.0E8 | -900 | see note* |
| A42039a_a01 | TrAa01ScC | $CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CHOCOO^- + H_2O_2$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |
| A42039b_a01 | TrAa01ScC | $CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2\ HCHO + 2\ CO_2 + H_2O_2 + 2\ OH^-$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |
| A42039c_a01 | TrAa01ScC | $CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CH_2OHCO_2^-$ | 0.30 × 7.50E7 | | Schuchmann et al. (1985) |
| A42039d_a01 | TrAa01ScC | $CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2\ CHOHOOCOO_2^-$ | 0.10 × 7.50E7 | | Schuchmann et al. (1985) |
| A42040_a01 | TrAa01ScC | $CH_2OOCO_2^- + O_3 \rightarrow O_3^- + HOCH_2OOH + CO_2$ | 2.00E9 | | Sehested et al. (1984) |
| A42141_a01 | TrAa01ScC | $HOOCCOO^- + OH \rightarrow C_2O_4^- + H_2O$ | 2.086E+08 | -2800 | Ervens et al. (2003) |
| A42142_a01 | TrAa01ScC | $C_2O_4^{2-} + OH \rightarrow C_2O_4^- + OH^-$ | 2.508E+08 | -4300 | Ervens et al. (2003) |
| A42143_a01 | TrAa01ScC | $C_2O_4^- + O_2 \rightarrow 2\ CO_2 + O_2^-$ | 2.40E9 | | Hislop and Bolton (1999) |
| A42144a_a01 | TrAa01ScC | $HOOCH2CO2H + OH \rightarrow CH_2OOCOOH + H_2O$ | 0.80 × 5.80E8 | | see note* |
| A42144b_a01 | TrAa01ScC | $HOOCH2CO2H + OH \rightarrow CHOOHOOCOOH + H_2O$ | 0.20 × 5.80E8 | | see note* |
| A42145a_a01 | TrAa01ScCN | $HOOCH2CO2H + NO_3 \rightarrow CH_2OOCOOH + NO_3^- + H^+$ | 0.80 × 1.70E6 | | Herrmann and Zellner (1998) |
| A42145b_a01 | TrAa01ScCN | $HOOCH2CO2H + NO_3 \rightarrow CHOOHOOCOOH + NO_3^- + H^+$ | 0.20 × 1.70E6 | | Herrmann and Zellner (1998) |
| A42146a_a01 | TrAa01ScC | $CH_2OOHCO_2^- + OH \rightarrow CH_2OOCO_2^- + H_2O$ | 0.80 × 5.80E8 | | see note* |
| A42146b_a01 | TrAa01ScC | $CH_2OOHCO_2^- + OH \rightarrow CHOOHOOCO_2^- + H_2O$ | 0.20 × 5.80E8 | | see note* |
| A42147a_a01 | TrAa01ScCN | $CH_2OOHCO_2^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$ | 0.80 × 7.10E6 | | Herrmann and Zellner (1998) |
| A42147b_a01 | TrAa01ScCN | $CH_2OOHCO_2^- + NO_3 \rightarrow CHOOHOOCO_2^- + NO_3^- + H^+$ | 0.20 × 7.10E6 | | Herrmann and Zellner (1998) |
| A42148_a01 | TrAa01ScC | $CHOOHOOCOOH \rightarrow HOOCCOOH + HO_2$ | 1.90E2 | | see note* |
| A42149_a01 | TrAa01ScC | $CHOOHOOCO_2^- \rightarrow HOOCCOO^- + HO_2$ | 1.90E2 | | see note* |
| A42150a_a01 | TrAa01ScC | $HOCH_2CO_2H + OH \rightarrow CHOHOOCOOH + H_2O$ | 0.62 × 6.00E8 | | see note* |
| A42150b_a01 | TrAa01ScC | $HOCH_2CO_2H + OH \rightarrow HCHO + CO_2 + HO_2 + H_2O$ | 0.38 × 6.00E8 | | see note* |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A42151a_a01 | TrAa01ScCN | $HOCH_2CO_2H + NO_3 \rightarrow CHOHOOCOOH + NO_3^- + H^+$ | 0.62 × 7.445E+05 | -3969 | see note* |
| A42151b_a01 | TrAa01ScCN | $HOCH_2CO_2H + NO_3 \rightarrow HCHO + CO_2 + HO_2 + NO_3^- + H^+$ | 0.38 × 7.445E+05 | -3969 | see note* |
| A42152_a01 | TrAa01ScC | $CHOHOOCOOH \rightarrow CHOCOOH + HO_2$ | 1.90E2 | | von Sonntag (1987) |
| A42153a_a01 | TrAa01ScC | $CH_2OHCO_2^- + OH \rightarrow CHOHOOCOO_2^- + H_2O$ | 0.60 × 8.60E8 | | Buxton et al. (1988) |
| A42153b_a01 | TrAa01ScC | $CH_2OHCO_2^- + OH \rightarrow HCHO + CO_2 + O_2^- + H_2O$ | 0.19 × 8.60E8 | | Buxton et al. (1988) |
| A42153c_a01 | TrAa01ScC | $CH_2OHCO_2^- + OH \rightarrow HOCH_2O_2 + CO_2 + OH^-$ | 0.21 × 8.60E8 | | Buxton et al. (1988) |
| A42154a_a01 | TrAa01ScCN | $CH_2OHCO_2^- + NO_3 \rightarrow CHOHOOCOO_2^- + NO_3^- + H^+$ | 0.76 × 7.502E+06 | -3007 | Gaillard de Sémainville et al. (2007) |
| A42154b_a01 | TrAa01ScCN | $CH_2OHCO_2^- + NO_3 \rightarrow HCHO + CO_2 + O_2^- + NO_3^- + H^+$ | 0.24 × 7.502E+06 | -3007 | Gaillard de Sémainville et al. (2007) |
| A42155_a01 | TrAa01ScC | $CHOHOOCOO_2^- \rightarrow CHOCOO^- + HO_2$ | 1.90E2 | | von Sonntag (1987) |
| A42156a_a01 | TrAa01ScC | $CHOOHOHCOOH + OH \rightarrow COOHCOHOHO_2 + H_2O$ | 0.15 × 2.830E+08 | -1000 | Ervens et al. (2003) |
| A42156b_a01 | TrAa01ScC | $CHOOHOHCOOH + OH \rightarrow HCOOH + CO_2 + HO_2 + H_2O$ | 0.85 × 2.830E+08 | -1000 | Ervens et al. (2003)* |
| A42157a_a01 | TrAa01ScCN | $CHOOHOHCOOH + NO_3 \rightarrow COOHCOHOHO_2 + NO_3^- + H^+$ | 0.15 × 1.00E6 | | see note* |
| A42157b_a01 | TrAa01ScCN | $CHOOHOHCOOH + NO_3 \rightarrow HCOOH + CO_2 + HO_2 + NO_3^- + H^+$ | 0.85 × 1.00E6 | | see note* |
| A42158a_a01 | TrAa01ScC | $CHOHOHCO_2^- + OH \rightarrow CO2^-COHOHO_2 + H_2O$ | 0.26 × 3.271E+09 | -4300 | Ervens et al. (2003) |
| A42158b_a01 | TrAa01ScC | $CHOHOHCO_2^- + OH \rightarrow HCOOH + CO_2 + O_2^- + H_2O$ | 0.74 × 3.271E+09 | -4300 | Ervens et al. (2003) |
| A42159a_a01 | TrAa01ScCN | $CHOHOHCO_2^- + NO_3 \rightarrow CO2^-COHOHO_2 + NO_3^- + H^+$ | 0.26 × 1.80E5 | | Herrmann and Zellner (1998) |
| A42159b_a01 | TrAa01ScCN | $CHOHOHCO_2^- + NO_3 \rightarrow HCOOH + CO_2 + O_2^- + NO_3^- + H^+$ | 0.74 × 1.80E5 | | Herrmann and Zellner (1998) |
| A42160_a01 | TrAa01ScC | $CHOHOHCO_2^- + H_2O_2 \rightarrow HCOO^- + CO_2 + H_2O + H_2O$ | 1.10E-1 | | Schöne and Herrmann (2014) |
| A42161_a01 | TrAa01ScC | $COOHCOHOHO_2 \rightarrow HOOCCOOH + HO_2$ | 1.00E6 | | see note* |
| A42162_a01 | TrAa01ScC | $CO2^-COHOHO_2 \rightarrow HOOCCOO^- + HO_2$ | 1.00E6 | | see note* |
| A42163a_a01 | TrAa01ScC | $CH_2OOHCHO + OH \rightarrow HCHO + CO + OH + H_2O$ | 0.77 × 1.40E9 | | see note* |
| A42163b_a01 | TrAa01ScC | $CH_2OOHCHO + OH \rightarrow GLYOX + HO_2 + H_2O$ | 0.23 × 1.40E9 | | see note* |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A42164a_a01 | TrAa01ScCN | $CH_2OOHCHO + NO_3 \rightarrow HCHO + CO + NO_3 + H_2O$ | 0.77 × 3.10E6 | | see note* |
| A42164b_a01 | TrAa01ScCN | $CH_2OOHCHO + NO_3 \rightarrow GLYOX + NO_3^- + H_2O + H^+$ | 0.23 × 3.10E6 | | see note* |
| A42165a_a01 | TrAa01ScC | $HOOCH_2CHOHOH + OH \rightarrow HOOCH2CO2H + HO_2 + H_2O$ | 0.33 × 1.10E9 | | see note* |
| A42165b_a01 | TrAa01ScC | $HOOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + OH + H_2O$ | 0.28 × 1.10E9 | | see note* |
| A42165c_a01 | TrAa01ScC | $HOOCH_2CHOHOH + OH \rightarrow HCOOH + HCHO + OH + H_2O$ | 0.39 × 1.10E9 | | see note* |
| A42166a_a01 | TrAa01ScCN | $HOOCH_2CHOHOH + NO_3 \rightarrow HOOCH2CO2H + NO_3^- + H_2O + H^+$ | 0.33 × 1.10E6 | | see note* |
| A42166b_a01 | TrAa01ScCN | $HOOCH_2CHOHOH + NO_3 \rightarrow CHOCHOHOH + NO_3 + H_2O$ | 0.28 × 1.10E6 | | see note* |
| A42166c_a01 | TrAa01ScCN | $HOOCH_2CHOHOH + NO_3 \rightarrow HCOOH + HCHO + NO_3 + H_2O$ | 0.39 × 1.10E6 | | see note* |
| A42167_a01 | TrAa01ScC | $HOCH_2OH + HOCH_2OH \rightarrow MG2 + H_2O$ | see note | see note | Hahnenstein et al. (1995)* |
| A42168_a01 | TrAa01ScC | $MG2 + H_2O \rightarrow HOCH_2OH + HOCH_2OH$ | see note | see note | Hahnenstein et al. (1995) |
| A42169_a01 | TrAa01ScC | $MG2 + OH \rightarrow HMF + HO_2$ | 1.54E9 | -1020 | see note* |
| A42470_a01 | TrAa01ScC | $CH_3COOO + H_2O \rightarrow CH_3COOH + HO_2$ | 7.0E5 | | Villalta et al. (1996) |
| A42471_a01 | TrAa01ScC | $CH_2OHCO3 + H_2O \rightarrow HOCH_2CO_2H + HO_2$ | 7.0E5 | | see note* |
| A42472_a01 | TrAa01ScC | $CHOCO_3 + H_2O \rightarrow CHOCOOH + HO_2$ | 7.0E5 | | see note* |
| A42473_a01 | TrAa01ScC | $COOHCO_3 + H_2O \rightarrow HOOCCOOH + HO_2$ | 7.0E5 | | see note* |
| A43000a_a01 | TrAa01ScC | $CH_3COCHOHOH + OH \rightarrow CH_3COCOOH + HO_2$ | 0.29 × 9.215E+08 | -1235 | Schaefer et al. (2015)* |
| A43000b_a01 | TrAa01ScC | $CH_3COCHOHOH + OH \rightarrow HCOOH + CH_3COOO$ | 0.71 × 9.215E+08 | -1235 | Schaefer et al. (2015) |
| A43001_a01 | TrAa01ScCN | $CH_3COCHOHOH + NO_3 \rightarrow CH_3COCOOH + NO_3^- + H^+$ | 4.539E+06 | -4213 | Schaefer et al. (2015)* |
| A43002_a01 | TrAa01ScC | $CH_3COCOOH + OH \rightarrow CH_3COOH + HO_2 + CO_2$ | 2.592E+08 | -1804 | Schaefer et al. (2012)* |
| A43003_a01 | TrAa01ScCN | $CH_3COCOOH + NO_3 \rightarrow CH_3COOH + NO_3^- + CO_2 + H^+$ | 2.828E+06 | -1804 | Gaillard de Sémainville et al. (2007) |
| A43004_a01 | TrAa01ScC | $CH_3COCO2^- + OH \rightarrow CH_3COO^- + HO_2 + CO_2$ | 6.252E+08 | -3007 | Schaefer et al. (2012)* |
| A43005_a01 | TrAa01ScCN | $CH_3COCO2^- + NO_3 \rightarrow CH_3COO^- + NO_3^- + CO_2 + H^+$ | 2.306E+07 | -2887 | Gaillard de Sémainville et al. (2007) |
| A43006_a01 | TrAa01ScC | $CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2$ | 1.80E8 | | Gligorovski et al. (2009) |
| A43007_a01 | TrAa01ScCN | $CH_3COCH_3 + NO_3 \rightarrow CH_3COCH_2O_2 + NO_3^- + H^+$ | 3.721E+03 | -4332 | Herrmann and Zellner (1998) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A43008a_a01 | TrAa01ScC | $CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow CH_3COCH_2OH + CH_3C(O)CHO$ | 0.20 × 4.00E8 | | Zegota et al. (1986) |
| A43008b_a01 | TrAa01ScC | $CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0\ CH_3C(O)CHO + H_2O_2$ | 0.45 × 4.00E8 | | Zegota et al. (1986) |
| A43009c_a01 | TrAa01ScC | $CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0\ HCHO + 2.0\ CH_3COOO$ | 0.15 × 4.00E8 | | Zegota et al. (1986) |
| A43009d_a01 | TrAa01ScC | $CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0\ CH_3C(O)CHO + 2.0\ HO_2$ | 0.20 × 4.00E8 | | Zegota et al. (1986) |
| A43010a_a01 | TrAa01ScC | $CH_3COCH_2OH + OH \rightarrow CH_3COCHOHO_2$ | 0.85 × 5.10E8 | | Doussin and Monod (2013)* |
| A43010b_a01 | TrAa01ScC | $CH_3COCH_2OH + OH \rightarrow HCHO + CH_3COOO$ | 0.15 × 5.10E8 | | Doussin and Monod (2013) |
| A43011_a01 | TrAa01ScCN | $CH_3COCH_2OH + NO_3 \rightarrow CH_3COCHOHO_2 + NO_3^- + H^+$ | 2.108E+07 | -1564 | Gaillard de Sémainville et al. (2007) |
| A43012_a01 | TrAa01ScC | $CH_3COCHOHO_2 \rightarrow CH_3C(O)CHO + HO_2$ | 1.90E2 | | von Sonntag (1987) |
| A43013_a01 | TrAa01ScC | $IPROPOL + OH \rightarrow CH_3COCH_3 + HO_2$ | 1.90E9 | | see note* |
| A43014_a01 | TrAa01ScCN | $IPROPOL + NO_3 \rightarrow CH_3COCH_3 + NO_3^- + H^+ + HO_2$ | 3.70E6 | | see note* |
| A43015a_a01 | TrAa01ScC | $CH_3COCH_2O_2H + OH \rightarrow CH_3C(O)CHO + OH$ | 1.80E8 | | see note* |
| A43015b_a01 | TrAa01ScC | $CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2$ | 4.70E8 | | see note* |
| A43016_a01 | TrAa01ScCN | $CH_3COCH_2O_2H + NO_3 \rightarrow CH_3COCH_2O_2 + NO_3^- + H^+$ | 4.50E6 | | see note* |
| A43017_a01 | TrAa01ScC | $CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$ | 4.30E5 | | see note* |
| A43018_a01 | TrAa01ScC | $CH_3COCH_2O_2 + O_2^- \rightarrow CH_3COCH_2O_2H + O_2 + OH^-$ | 5.00E7 | | see note* |
| A43019a_a01 | TrAa01ScC | $iC_3H_7OOH + OH \rightarrow CH_3COCH_3 + OH$ | 9.90E8 | | see note* |
| A43019b_a01 | TrAa01ScC | $iC_3H_7OOH + OH \rightarrow iC_3H_7O_2$ | 1.80E8 | | see note* |
| A43020_a01 | TrAa01ScCN | $iC_3H_7OOH + NO_3 \rightarrow iC_3H_7O_2 + NO_3^- + H^+$ | 4.50E6 | | see note* |
| A43021_a01 | TrAa01ScC | $iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$ | 4.30E5 | | see note* |
| A43022_a01 | TrAa01ScC | $iC_3H_7O_2 + O_2^- \rightarrow iC_3H_7OOH + O_2 + OH^-$ | 5.00E7 | | see note* |
| A43023_a01 | TrAa01ScC | $HOCH_2OH + MG2 \rightarrow MG3 + H_2O$ | see note | see note | Hahnenstein et al. (1995)* |
| A43024_a01 | TrAa01ScC | $MG3 + H_2O \rightarrow HOCH_2OH + MG2$ | see note | see note | Hahnenstein et al. (1995) |
| A43025_a01 | TrAa01ScC | $MG3 + OH \rightarrow HM2F + HO_2$ | 1.54E9 | -1020 | see note* |
| A44000_a01 | TrAa01ScC | $MACR + OH \rightarrow CH_2OHCO_2CH_3CHO$ | 9.905E+09 | -1203 | Schöne and Herrmann (2014) |
| A44001_a01 | TrAa01ScC | $CH_2OHCO_2CH_3CHO + CH_2OHCO_2CH_3CHO \rightarrow CH_3C(O)CHO + CH_3COCH_2OH + HOCH_2O_2 + HCOHOHO_2$ | 4.00E8 | | Schöne and Herrmann (2014) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A44002_a01 | TrAa01ScC | MVK + OH → $CH_3COCHO_2CH_2OH$ | 7.117E+09 | -1443 | Schöne and Herrmann (2014) |
| A44003_a01 | TrAa01ScC | $CH_3COCHO_2CH_2OH$ + $CH_3COCHO_2CH_2OH$ → 1.1 $CH_2COCOCH_2OH$ + .2 $CH_2OHCHOOHCOCH_3$ + .35 $CH_2OHCHO$ + .35 $CH_3C(O)CHO$ + .35 $HOCH_2O_2$ + .35 $CH_3COOO$ + .45 $H_2O_2$ | 4.00E8 | | Schöne and Herrmann (2014) |
| A44004_a01 | TrAa01ScC | GLYOX + CHOCHOHOH → GOLIG1 + $H_2O$ | 1.00E2 | | Ervens and Volkamer (2010) |
| A44005_a01 | TrAa01ScC | GOLIG1 + $H_2O$ → GLYOX + CHOCHOHOH | 1.00E-1 | | Ervens and Volkamer (2010) |
| A44006_a01 | TrAa01ScC | CHOCHOHOH + CHOCHOHOH → GOLIG2 + $H_2O$ | 1.00E2 | | Ervens and Volkamer (2010) |
| A44007_a01 | TrAa01ScC | GOLIG2 + $H_2O$ → CHOCHOHOH + CHOCHOHOH | 1.00E-1 | | Ervens and Volkamer (2010) |
| A44008_a01 | TrAa01ScC | CHOHOHCHOHOH + CHOCHOHOH → GOLIG3 + $H_2O$ | 1.00E2 | | Ervens and Volkamer (2010) |
| A44009_a01 | TrAa01ScC | GOLIG3 + $H_2O$ → CHOHOHCHOHOH + CHOCHOHOH | 1.00E-1 | | Ervens and Volkamer (2010) |
| A44010_a01 | TrAa01ScC | GOLIG1 + OH → GOLIGO1 + $HO_2$ | 1.610E+09 | -1516 | see note* |
| A44011_a01 | TrAa01ScC | GOLIG2 + OH → GOLIGO2 + $HO_2$ | 1.610E+09 | -1516 | see note* |
| A44012_a01 | TrAa01ScC | GOLIG3 + OH → GOLIGO3 + $HO_2$ | 1.610E+09 | -1516 | see note* |
| A46000_a01 | TrAa01ScC | $CH_3C(O)CHO$ + $CH_3COCHOHOH$ → $CH_3COCHOHOCHOHCOCH_3$ + $H_2O$ | 1.00E2 | | Ervens and Volkamer (2010)* |
| A46001_a01 | TrAa01ScC | $CH_3COCHOHOCHOHCOCH_3$ + $H_2O$ → $CH_3COCHOHOH$ + $CH_3C(O)CHO$ | 1.00E-1 | | Ervens and Volkamer (2010)* |
| A46002_a01 | TrAa01ScC | $CH_3COCHOHOCHOHCOCH_3$ + OH → $CH_3COCOHOCOHCOCH_3$ + $HO_2$ | 1.303E+09 | -1235 | see note* |
| A46003_a01 | TrAa01ScC | $CH_3COCHOHOH$ + $CH_3COCHOHOH$ → $CH_3COCHOHOCOHC_3CHOHOH$ + $H_2O$ | 1.00E2 | | Ervens and Volkamer (2010)* |
| A46004_a01 | TrAa01ScC | $CH_3COCHOHOCOHC_3CHOHOH$ + $H_2O$ → 2 $CH_3COCHOHOH$ | 1.00E-1 | | Ervens and Volkamer (2010)* |
| A46005_a01 | TrAa01ScC | $CH_3COCHOHOCOHC_3CHOHOH$ + OH → $CH_3COCOHOCOHC_3COHOH$ + $HO_2$ | 1.303E+09 | -1235 | see note* |
| A60000_a01 | TrAa01Cl | Cl + Cl → $Cl_2$ | 8.8E7 | | Wu et al. (1980) |
| A60001_a01 | TrAa01Cl | $Cl_2^-$ + $Cl_2^-$ → $Cl_2$ + 2 $Cl^-$ | 3.5E9 | | Yu (2004) |
| A61000_a01 | TrAa01Cl | $Cl^-$ + $O_3$ → $ClO^-$ | 3.0E-3 | | Hoigné et al. (1985) |
| A61001_a01 | TrAa01Cl | $Cl_2$ + $O_2^-$ → $Cl_2^-$ | 1.0E9 | | Bjergbakke et al. (1981) |
| A61002_a01 | TrAa01Cl | $Cl_2^-$ + $O_2^-$ → 2 $Cl^-$ | 1.0E9 | | Jacobi (1996)* |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A62000_a01 | TrAa01Cl | $Cl \rightarrow H^+ + ClOH^-$ | 1.8E5 | | Yu (2004) |
| A62001_a01 | TrAa01Cl | $Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$ | 2.7E7 | -1684 | Christensen et al. (1982) |
| A62002_a01 | TrAa01Cl | $Cl^- + OH \rightarrow ClOH^-$ | 4.2E9 | | Yu (2004) |
| A62003_a01 | TrAa01Cl | $Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$ | 1.0E9 | | Bjergbakke et al. (1981) |
| A62004_a01 | TrAa01MblCl | $Cl_2 \rightarrow Cl^- + HOCl + H^+$ | 21.8 | -8012 | Wang and Margerum (1994) |
| A62005_a01 | TrAa01Cl | $Cl_2^- + HO_2 \rightarrow 2\ Cl^- + H^+$ | 1.3E10 | | Jacobi (1996) |
| A62006_a01 | TrAa01Cl | $HOCl + O_2^- \rightarrow Cl + OH^-$ | 7.5E6 | | Long and Bielski (1980) |
| A62007_a01 | TrAa01Cl | $HOCl + HO_2 \rightarrow Cl$ | 7.5E6 | | Long and Bielski (1980) |
| A62008_a01 | TrAa01MblCl | $HOCl + Cl^- + H^+ \rightarrow Cl_2$ | 2.2E4 | -3508 | Wang and Margerum (1994) |
| A62009_a01 | TrAa01Cl | $ClOH^- \rightarrow Cl^- + OH$ | 6.0E9 | | Yu (2004) |
| A62010_a01 | TrAa01Cl | $ClOH^- + H^+ \rightarrow Cl$ | 2.4E10 | | Yu (2004) |
| A63000_a01 | TrAa01ClN | $Cl + NO_3^- \rightarrow NO_3 + Cl^-$ | 1.0E8 | | Buxton et al. (1999b) |
| A63001_a01 | TrAa01ClN | $Cl^- + NO_3 \rightarrow NO_3^- + Cl$ | 3.4E8 | | Buxton et al. (1999b)* |
| A63002_a01 | TrAa01ClN | $Cl_2^- + NO_2^- \rightarrow 2\ Cl^- + NO_2$ | 6.0E7 | | Jacobi et al. (1996) |
| A64000_a01 | TrAa01ScCl | $Cl_2^- + CH_3OOH \rightarrow 2\ Cl^- + H^+ + CH_3OO$ | 6.20E5 | | see note* |
| A70000_a01 | TrAa01Br | $Br_2^- + Br_2^- \rightarrow 2\ Br^- + Br_2$ | 1.9E9 | | Ross et al. (1992) |
| A71000_a01 | TrAa01Br | $Br^- + O_3 \rightarrow BrO^-$ | 2.1E2 | -4450 | Haag and Hoigné (1983) |
| A71001_a01 | TrAa01Br | $Br_2 + O_2^- \rightarrow Br_2^-$ | 5.6E9 | | Sutton and Downes (1972) |
| A71002_a01 | TrAa01Br | $Br_2^- + O_2^- \rightarrow 2\ Br^-$ | 1.7E8 | | Wagner and Strehlow (1987) |
| A72000_a01 | TrAa01Br | $Br^- + OH \rightarrow BrOH^-$ | 1.1E10 | | Zehavi and Rabani (1972) |
| A72001_a01 | TrAa01Br | $Br_2 + HO_2 \rightarrow Br_2^- + H^+$ | 1.1E8 | | Sutton and Downes (1972) |
| A72002_a01 | TrAa01MblBr | $Br_2 \rightarrow Br^- + HOBr + H^+$ | 9.7E1 | -7457 | Beckwith et al. (1996) |
| A72003_a01 | TrAa01Br | $Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$ | 4.4E9 | | Matthew et al. (2003) |
| A72004_a01 | TrAa01Br | $Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$ | 1.0E5 | | Jacobi (1996) |
| A72005_a01 | TrAa01Br | $HOBr + O_2^- \rightarrow Br + OH^-$ | 3.5E9 | | Schwarz and Bielski (1986) |
| A72006_a01 | TrAa01Br | $HOBr + HO_2 \rightarrow Br$ | 1.0E9 | | Herrmann et al. (1999a) |
| A72007_a01 | TrAa01Br | $HOBr + H_2O_2 \rightarrow Br^- + H^+$ | 1.2E6 | | Bichsel and von Gunten (1999) |
| A72008_a01 | TrAa01MblBr | $HOBr + Br^- + H^+ \rightarrow Br_2$ | 1.6E10 | | Beckwith et al. (1996) |
| A72009a_a01 | TrAa01Br | $BrOH^- \rightarrow Br^- + OH$ | 3.3E7 | | Zehavi and Rabani (1972) |
| A72009b_a01 | TrAa01Br | $BrOH^- \rightarrow Br + OH^-$ | 4.2E6 | | Zehavi and Rabani (1972) |
| A72010_a01 | TrAa01Br | $BrOH^- + H^+ \rightarrow Br$ | 4.4E10 | | Zehavi and Rabani (1972) |
| A73000_a01 | TrAa01BrN | $Br^- + NO_3 \rightarrow Br + NO_3^-$ | 4.0E9 | | Neta and Huie (1986) |
| A73001_a01 | TrAa01BrN | $Br_2^- + NO_2^- \rightarrow 2\ Br^- + NO_2$ | 1.7E7 | -1720 | Shoute et al. (1991) |
| A74000_a01 | TrAa01Br | $Br_2^- + CH_3OOH \rightarrow 2\ Br^- + H^+ + CH_3OO$ | 1.0E5 | | Jacobi (1996)* |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A76001_a01 | TrAa01BrCl | $Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$ | 3.7E10 | | Kumar and Margerum (1987) |
| A76002_a01 | TrAa01MblBrCl | $Br^- + HOCl + H^+ \rightarrow BrCl$ | 1.32E6 | | Kumar and Margerum (1987) |
| A76003_a01 | TrAa01MblBrCl | $HOBr + Cl^- + H^+ \rightarrow BrCl$ | 2.3E10 | | Liu and Margerum (2001)* |
| A76004_a01 | TrAa01MblBrCl | $BrCl \rightarrow Cl^- + HOBr + H^+$ | 3.0E6 | | Liu and Margerum (2001) |
| A81000_a01 | TrAa01MblI | $I^- + O_3 \rightarrow HOI + OH^-$ | 4.2E9 | -9311 | Magi et al. (1997) |
| A81001_a01 | TrAa01MblI | $IO + IO \rightarrow HOI + IO_2^- + H^+$ | 1.5E9 | | Buxton et al. (1986) |
| A82000_a01 | TrAa01MblI | $IO_2^- + H_2O_2 \rightarrow IO_3^-$ | 6.0E1 | | Furrow (1987) |
| A82001_a01 | TrAa01I | $HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$ | 6.0E2 | | Chinake and Simoyi (1996) |
| A82002_a01 | TrAa01MblI | $HOI + I^- + H^+ \rightarrow I_2$ | 4.4E12 | | Eigen and Kustin (1962) |
| A82003_a01 | TrAa01MblI | $IO_2^- + I^- + H^+ \rightarrow 2\ HOI + OH^-$ | 2.0E10 | | Edblom et al. (1987) |
| A86000_a01 | TrAa01MblClI | $ICl \rightarrow HOI + Cl^- + H^+$ | 2.4E6 | | Wang et al. (1989) |
| A86001_a01 | TrAa01MblClI | $I^- + HOCl + H^+ \rightarrow ICl$ | 3.5E11 | | Nagy et al. (1988) |
| A86002_a01 | TrAa01ClI | $IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$ | 1.5E3 | | Lengyel et al. (1996) |
| A86003_a01 | TrAa01MblClI | $HOI + Cl^- + H^+ \rightarrow ICl$ | 2.9E10 | | Wang et al. (1989) |
| A86004_a01 | TrAa01ClI | $HOI + Cl_2 \rightarrow IO_2^- + 2\ Cl^- + 3H^+$ | 1.0E6 | | Lengyel et al. (1996) |
| A86005_a01 | TrAa01ClI | $HOI + HOCl \rightarrow IO_2^- + Cl^- + 2\ H^+$ | 5.0E5 | | Citri and Epstein (1988) |
| A86006_a01 | TrAa01ClI | $ICl + I^- \rightarrow I_2 + Cl^-$ | 1.1E9 | | Margerum et al. (1986) |
| A87000_a01 | TrAa01MblBrI | $IBr \rightarrow HOI + H^+ + Br^-$ | 8.0E5 | | Troy et al. (1991) |
| A87001_a01 | TrAa01MblBrI | $I^- + HOBr \rightarrow IBr + OH^-$ | 5.0E9 | | Troy and Margerum (1991) |
| A87002_a01 | TrAa01BrI | $IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$ | 1.0E6 | | Chinake and Simoyi (1996) |
| A87003_a01 | TrAa01MblBrI | $HOI + Br^- + H^+ \rightarrow IBr$ | 3.3E12 | | Troy et al. (1991) |
| A87004_a01 | TrAa01BrI | $HOI + HOBr \rightarrow IO_2^- + Br^- + 2\ H^+$ | 1.0E6 | | Chinake and Simoyi (1996) |
| A87005_a01 | TrAa01BrI | $IBr + I^- \rightarrow I_2 + Br^-$ | 2.0E9 | | Faria et al. (1993) |
| A91000_a01 | TrAa01ScS | $SO_3^- + O_2 \rightarrow SO_5^-$ | 1.5E9 | | Huie and Neta (1987) |
| A91001_a01 | TrAa01MblScScmS | $SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$ | 1.5E9 | -5300 | Hoffmann (1986) |
| A91002_a01 | TrAa01ScS | $SO_4^- + O_2^- \rightarrow SO_4^{2-}$ | 3.5E9 | | Jiang et al. (1992) |
| A91003_a01 | TrAa01ScS | $SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$ | 4.6E8 | | Huie and Neta (1987) |
| A91004_a01 | TrAa01ScS | $SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$ | 2.3E8 | | Buxton et al. (1996) |
| A91005_a01 | TrAa01S | $SO_5^- + SO_3^{2-} \rightarrow .72\ SO_4^- + .72\ SO_4^{2-} + .28\ SO_3^- + .28\ HSO_5^- + .28\ OH^-$ | 1.3E7 | | Huie and Neta (1987), Deister and Warneck (1990)* |
| A91006_a01 | TrAa01S | $SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + LSULFUR$ | 1.0E8 | | Ross et al. (1992)* |
| A92000_a01 | TrAa01ScS | $SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$ | 5.5E9 | | Buxton et al. (1988) |
| A92001_a01 | TrAa01ScS | $SO_4^- + OH \rightarrow HSO_5^-$ | 1.0E9 | | Jiang et al. (1992) |
| A92002_a01 | TrAa01ScS | $SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$ | 3.5E9 | | Jiang et al. (1992) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A92003_a01 | TrAa01ScS | $SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$ | 1.1E1 | -1110 | Herrmann et al. (1995) |
| A92004_a01 | TrAa01ScS | $SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$ | 1.2E7 | | Wine et al. (1989) |
| A92005_a01 | TrAa01ScS | $HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$ | 3.0E3 | | see note* |
| A92006_a01 | TrAa01MblScScmS | $HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$ | 3.7E5 | -5500 | Hoffmann (1986) |
| A92007_a01 | TrAa01ScS | $HSO_3^- + OH \rightarrow SO_3^-$ | 4.5E9 | | Buxton et al. (1988) |
| A92008_a01 | TrAa01ScS | $HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$ | 3.0E3 | | see note* |
| A92009_a01 | TrAa01MblScScmS | $HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$ | 5.2E6 | -3650 | Martin and Damschen (1981) |
| A92010_a01 | TrAa01ScS | $HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$ | 8.0E8 | | Huie and Neta (1987) |
| A92011_a01 | TrAa01S | $HSO_3^- + SO_5^- \rightarrow .75\ SO_4^- + .75\ SO_4^{2-} + .75\ H^+ + .25\ SO_3^- + .25\ HSO_5^-$ | 1.0E5 | | Huie and Neta (1987) |
| A92012_a01 | TrAa01ScS | $HSO_3^- + HSO_5^- + H^+ \rightarrow 2\ HSO_4^- + H^+$ | 7.1E6 | | Betterton and Hoffmann (1988) |
| A93001_a01 | TrAa01ScNS | $SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$ | 5.0E4 | | Exner et al. (1992) |
| A93002_a01 | TrAa01ScNS | $SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$ | 1.0E5 | | Løgager et al. (1993) |
| A93004_a01 | TrAa01ScNS | $HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$ | 1.4E9 | -2000 | Exner et al. (1992) |
| A93005_a01 | TrAa01ScNS | $HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$ | 3.1E5 | | Warneck (1999) |
| A94100_a01 | TrAa01ScS | $SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$ | 1.4E4 | | Boyce and Hoffmann (1984)* |
| A94101_a01 | TrAa01ScS | $SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$ | 1.6E7 | -3800 | Lind et al. (1987) |
| A94102_a01 | TrAa01ScS | $HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$ | 4.3E-1 | | Boyce and Hoffmann (1984)* |
| A94103_a01 | TrAa01ScS | $HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$ | 1.6E7 | -3800 | Lind et al. (1987) |
| A94104_a01 | TrAa01ScS | $HSO_3^- + CH_3OO \rightarrow SO_3^- + CH_3OOH$ | 5.00E5 | | Herrmann et al. (1999b) |
| A94105_a01 | TrAa01ScS | $SO_4^- + HCOO^- \rightarrow SO_4^{2-} + CO_2 + HO_2$ | 1.7E8 | -1500 | Jacob (1986) |
| A94106_a01 | TrAa01ScS | $SO_4^- + HCOOH \rightarrow SO_4^{2-} + CO_2 + H^+ + HO_2$ | 1.7E8 | -1500 | Jacob (1986) |
| A94107_a01 | TrAa01ScS | $SO_4^- + CH_3OH \rightarrow SO_4^{2-} + HOCH_2O_2 + H^+$ | 9.039E+06 | -2190 | Clifton and Huie (1989) |
| A94108a_a01 | TrAa01ScS | $SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + CH_3OO + H^+$ | 0.25 × 1.20E7 | | see note* |
| A94108b_a01 | TrAa01ScS | $SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + HCHO + HO_2 + H^+$ | 0.75 × 1.20E7 | | see note* |
| A94109_a01 | TrAa01ScS | $SO_4^- + HOCH_2OH \rightarrow SO_4^{2-} + HCOHOHO_2 + H^+$ | 1.40E7 | -1300 | Buxton et al. (1990) |
| A94110_a01 | TrAa01ScS | $SO_5^- + HCOO^- \rightarrow HSO_5^- + CO_2 + O_2^-$ | 1.4E4 | -4000 | Jacob (1986) |
| A94111_a01 | TrAa01ScS | $CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$ | 3.6E3 | | Seinfeld and Pandis (1998) |
| A94200_a01 | TrAa01ScCS | $HSO_3^- + CH_2OOCOOH \rightarrow SO_3^- + HOOCH2CO2H$ | 5.00E5 | | see note* |
| A94201_a01 | TrAa01ScCS | $HSO_3^- + CH_2OOCO_2^- \rightarrow SO_3^- + CH_2OOHCO_2^-$ | 5.00E5 | | see note* |
| A94202a_a01 | TrAa01ScCS | $SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_3CHO + HO_2 + H^+$ | 0.90 × 4.236E+07 | -1750 | Clifton and Huie (1989)* |
| A94202b_a01 | TrAa01ScCS | $SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_2OHCH_2OO + H^+$ | 0.10 × 4.236E+07 | -1750 | Clifton and Huie (1989) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A94203a_a01 | TrAa01ScCS | $SO_4^- + CHOHOHCHOHOH \rightarrow SO_4^{2-} + CHOHOHCOHOHO_2 + H^+$ | 0.27 × 2.40E7 | | George et al. (2001) |
| A94203b_a01 | TrAa01ScCS | $SO_4^- + CHOHOHCHOHOH \rightarrow SO_4^{2-} + HCOHOHO_2 + HCOOH + HO_2 + H^+$ | 0.73 × 2.40E7 | | George et al. (2001)* |
| A94204_a01 | TrAa01ScCS | $SO_4^- + CH_3COO^- \rightarrow SO_4^{2-} + CH_2OOCO_2^- + H^+$ | 5.10E6 | | Huie and Clifton (1990) |
| A94205_a01 | TrAa01ScCS | $SO_4^- + HOOCCOO^- \rightarrow SO_4^{2-} + C_2O_4^- + H^+$ | 1.70E6 | | Grgić et al. (2007) |
| A94206_a01 | TrAa01ScCS | $SO_4^- + C_2O_4^{2-} \rightarrow SO_4^{2-} + C_2O_4^-$ | 1.30E7 | | Grgić et al. (2007) |
| A96000_a01 | TrAa01ClS | $SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2\ Cl^-$ | 6.2E7 | | Jacobi et al. (1996) |
| A96001_a01 | TrAa01MblClS | $SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$ | 7.6E8 | | Fogelman et al. (1989) |
| A96002_a01 | TrAa01ClS | $SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$ | 2.5E8 | | Buxton et al. (1999a) |
| A96003_a01 | TrAa01ClS | $SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$ | 2.1E8 | | Buxton et al. (1999a) |
| A96004_a01 | TrAa01ClS | $HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2\ Cl^- + H^+$ | 4.7E8 | -1082 | Shoute et al. (1991) |
| A96005_a01 | TrAa01MblClS | $HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$ | 7.6E8 | | see note* |
| A96006_a01 | TrAa01ClS | $HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$ | 1.8E-3 | -7352 | Fortnum et al. (1960) |
| A97000_a01 | TrAa01BrS | $SO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + SO_3^-$ | 2.2E8 | -649 | Shoute et al. (1991) |
| A97001_a01 | TrAa01BrS | $SO_3^{2-} + BrO^- \rightarrow Br^- + SO_4^{2-}$ | 1.0E8 | | Troy and Margerum (1991) |
| A97002_a01 | TrAa01MblBrS | $SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$ | 5.0E9 | | Troy and Margerum (1991) |
| A97003_a01 | TrAa01BrS | $SO_4^- + Br^- \rightarrow Br + SO_4^{2-}$ | 2.1E9 | | Jacobi (1996) |
| A97004_a01 | TrAa01BrS | $HSO_3^- + Br_2^- \rightarrow 2\ Br^- + H^+ + SO_3^-$ | 6.3E7 | -782 | Shoute et al. (1991) |
| A97005_a01 | TrAa01MblBrS | $HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$ | 5.0E9 | | see note* |
| A97006_a01 | TrAa01BrS | $HSO_5^- + Br^- \rightarrow HOBr + SO_4^{2-}$ | 1.0E0 | -5338 | Fogelman et al. (1989) |
| A98000_a01 | TrAa01IS | $HSO_3^- + I_2 \rightarrow 2\ I^- + HSO_4^- + 2\ H^+$ | 1.7E9 | | Yiin and Margerum (1990) |
| A101000_a01 | TrAa01Hg | $Hg + O_3 \rightarrow HgO + O_2$ | 4.7E7 | | Munthe (1992) |
| A102000_a01 | TrAa01Hg | $HgO + H^+ \rightarrow Hg^{2+} + OH^-$ | 1.0E10 | | Pleijel and Munthe (1995) |
| A102001_a01 | TrAa01Hg | $Hg + OH \rightarrow Hg^+ + OH^-$ | 2.0E9 | | Lin and Pehkonen (1997) |
| A102002_a01 | TrAa01Hg | $Hg^+ + OH \rightarrow Hg^{2+} + OH^-$ | 1.0E10 | | Lin and Pehkonen (1997) |
| A102003_a01 | TrAa01Hg | $Hg^{2+} + HO_2 \rightarrow Hg^+ + O_2 + H^+$ | 1.7E4 | | Enami et al. (2007) |
| A102004_a01 | TrAa01Hg | $Hg^+ + HO_2 \rightarrow Hg + O_2 + H^+$ | 1.0E10 | | Lin and Pehkonen (1997) |
| A106000_a01 | TrAa01ClHg | $Hg + HOCl \rightarrow Hg^{2+} + Cl^- + OH^-$ | 2.09E6 | | Lin and Pehkonen (1998) |
| A106001_a01 | TrAa01ClHg | $Hg + ClO^- \rightarrow Hg^{2+} + Cl^- + 2\ OH^-$ | 1.99E6 | | Lin and Pehkonen (1998) |
| A107000_a01 | TrAa01BrHg | $Hg + HOBr \rightarrow Hg^{2+} + Br^- + OH^-$ | 0.279 | | Wang and Pehkonen (2004) |
| A107001_a01 | TrAa01BrHg | $Hg + BrO^- \rightarrow Hg^{2+} + Br^- + 2\ OH^-$ | 0.273 | | Wang and Pehkonen (2004) |
| A107002_a01 | TrAa01BrHg | $Hg + Br_2 \rightarrow Hg^{2+} + 2\ Br^-$ | 0.196 | | Wang and Pehkonen (2004) |
| A109000_a01 | TrAa01HgS | $HgSO_3 \rightarrow Hg + HSO_4^- + H^+$ | 0.0106 | | van Loon et al. (2000) |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A111001_a01 | TrAa01Fe | $Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO2^- + OH^-$ | 1E7 | | de Laat and Le (2006) |
| A111002_a01 | TrAa01Fe | $Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$ | 5E7 | | de Laat and Le (2006) |
| A111003_a01 | TrAa01Fe | $Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$ | 8.2E5 | | Løgager et al. (1992) |
| A112001a_a01 | TrAa01Fe | $Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$ | 2.7E8 | | de Laat and Le (2006) |
| A112001b_a01 | TrAa01Fe | $FeOH^+ + OH \rightarrow Fe^{3+} + 2\ OH^-$ | 2.7E8 | | de Laat and Le (2006) |
| A112002a_a01 | TrAa01Fe | $Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$ | 5.5E1 | | de Laat and Le (2006) |
| A112002b_a01 | TrAa01Fe | $FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2\ OH^-$ | 5.9E6 | | de Laat and Le (2006) |
| A112003_a01 | TrAa01Fe | $FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$ | 2.3E-3 | | de Laat and Le (2006) |
| A112004_a01 | TrAa01Fe | $Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$ | 2.3E-3 | | de Laat and Le (2006) |
| A112006_a01 | TrAa01Fe | $Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO2^-$ | 1.2E6 | | de Laat and Le (2006) |
| A112008a_a01 | TrAa01Fe | $FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$ | 1.5E8 | | Rush and Bielski (1985) |
| A112008b_a01 | TrAa01Fe | $Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2\ OH^-$ | 1.5E8 | | Rush and Bielski (1985) |
| A112009_a01 | TrAa01Fe | $Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2\ OH^-$ | 1.0E7 | | Rush and Bielski (1985) |
| A112010_a01 | TrAa01Fe | $Fe^{2+} + OH \rightarrow FeOH^{2+}$ | 4.3E8 | | Christensen and Sehested (1981) |
| A112011_a01 | TrAa01Fe | $FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$ | 9.5E3 | | Løgager et al. (1992) |
| A112012_a01 | TrAa01Fe | $FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$ | 1.3E-2 | | Løgager et al. (1992) |
| A112013_a01 | TrAa01Fe | $FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$ | 2.0E6 | | Løgager et al. (1992) |
| A112014_a01 | TrAa01Fe | $FeO^{2+} + OH \rightarrow Fe^{3+} + HO2^-$ | 1.0E7 | | Løgager et al. (1992) |
| A112015_a01 | TrAa01Fe | $FeO^{2+} + Fe^{2+} \rightarrow 2\ Fe^{3+} + 2\ OH^-$ | 1.4E5 | | Løgager et al. (1992) |
| A112016_a01 | TrAa01Fe | $FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+}$ | 1.8E4 | | Jacobsen et al. (1997) |
| A112017_a01 | TrAa01Fe | $Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2\ Fe^{3+} + OH^-$ | 2.0 | | Jacobsen et al. (1997) |
| A112018_a01 | TrAa01Fe | $Fe(OH)_2Fe^{4+} \rightarrow 2\ Fe^{3+} + 2\ OH^-$ | 0.49 | | Jacobsen et al. (1997) |
| A113001_a01 | TrAa01FeN | $FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$ | 1.1E4 | | Jacobsen et al. (1998) |
| A113002_a01 | TrAa01FeN | $Fe^{2+} + NO_3 \rightarrow Fe^{3+} + NO_3^-$ | 8.0E6 | | Herrmann et al. (2000) |
| A116001_a01 | TrAa01ClFe | $Fe^{2+} + Cl \rightarrow Fe^{3+} + Cl^-$ | 5.9E9 | | Jayson et al. (1973) |
| A116002a_a01 | TrAa01ClFe | $Fe^{2+} + Cl_2^- \rightarrow Fe^{3+} + 2\ Cl^-$ | 1E7 | | Thornton and Laurence (1973) |
| A116002b_a01 | TrAa01ClFe | $Fe^{2+} + Cl_2^- \rightarrow FeCl^{2+} + Cl^-$ | 4E6 | | Thornton and Laurence (1973) |
| A116003a_a01 | TrAa01ClFe | $FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO2^-$ | 1.2E6 | | de Laat and Le (2006) |
| A116003b_a01 | TrAa01ClFe | $FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO2^- + OH^-$ | 1E7 | | de Laat and Le (2006) |
| A116004a_a01 | TrAa01ClFe | $FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$ | 2E4 | | de Laat and Le (2006) |
| A116004b_a01 | TrAa01ClFe | $FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2\ Cl^- + O_2 + H^+$ | 2E4 | | de Laat and Le (2006) |
| A116004c_a01 | TrAa01ClFe | $FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$ | 5E7 | | de Laat and Le (2006) |
| A116004d_a01 | TrAa01ClFe | $FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2\ Cl^- + O_2$ | 5E7 | | de Laat and Le (2006) |
| A116005_a01 | TrAa01ClFe | $FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2\ OH^-$ | 1E2 | | Jacobsen et al. (1998)* |

Table 6: Aqueous phase reactions (...continued)

| # | labels | reaction | $k_0$ $[M^{1-n}s^{-1}]$ | $-E_a/R[K]$ | reference |
|---|---|---|---|---|---|
| A117001_a01 | TrAa01BrFe | $Fe^{2+} + Br_2^- \rightarrow Fe^{3+} + 2\ Br^-$ | 3.6E6 | | Thornton and Laurence (1973) |
| A119001_a01 | TrAa01FeS | $FeO^{2+} + SO_2 \rightarrow Fe^{3+} + SO_3^-$ | 4.5E5 | | Jacobsen et al. (1998)* |
| A119002_a01 | TrAa01FeS | $FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH^-$ | 2.5E5 | | Jacobsen et al. (1998)* |
| A119003_a01 | TrAa01FeS | $FeOH^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$ | 30 | | Ziajka et al. (1994) |
| A119004_a01 | TrAa01FeS | $Fe^{2+} + SO_5^- \rightarrow FeOH^{2+} + HSO_5^-$ | 8E5 | | Ziajka et al. (1994)* |
| A119005_a01 | TrAa01FeS | $Fe^{2+} + HSO_5^- \rightarrow FeOH^{2+} + SO_4^-$ | 3.0E4 | | Gilbert and Stell (1990) |
| A119006_a01 | TrAa01FeS | $Fe^{2+} + SO_4^- \rightarrow FeSO_4^+$ | 3.6E7 | | McElroy and Waygood (1990)* |
| A119007_a01 | TrAa01FeS | $FeOH^{2+} + SO_3^- \rightarrow Fe^{2+} + HSO_4^-$ | 3E7 | | Warneck (2018) |
| A119008_a01 | TrAa01FeS | $FeSO_3^+ + SO_3^- \rightarrow Fe^{2+} + SO_4^{2-} + SO_2$ | 2.16E6 | | Warneck (2018)* |

## Specific notes

A41013a_a01: Branching ratios taken from Asmus et al. (1973)

A41016a_a01: Branching ratio explaining the HCOOH-yield by Monod et al. (2007) who originally assigned it to the channel for the methylic H-abstraction. However, Monod et al. (2007), differently from Herrmann et al. (1999b), assumed that the self-reaction of $CH_3O_2$ would only produce 2 $CH_3O$ radicals and thus HCHO + $HO_2$. Instead, the latter reaction has a 0.8 yield of $HOCH_2O_2$, which is a precursor of hydroxymethyl hydroperoxide and thus HCOOH.

A41016b_a01: The $CH_2OOH$ radical has a lifetime of $10^{-9}$ s in the gas phase decomposing to HCHO and OH. $O_2$-addition in the aqueous-phase seems unlikely. It is hard to imagine how the $HOOHCH_2O_2$ radical would decompose into HCOOH and $HO_2$.

A41017a_a01: $k(H_2O_2+NO_3)$, branching ratio as for $CH_3OOH$ + OH

A41017b_a01: See branch a.

A41018a_a01: $k(H_2O_2+CO_3^-)$, branching ratio as for $CH_3OOH$ + OH

A41018b_a01: See branch a.

A41019a_a01: Branching ratio as for $CH_3OOH$ + OH

A41019b_a01: $HOCHOOHO_2$ is assumed to directly decompose into CHOOOH and $HO_2$

A41020a_a01: $k(H_2O_2+NO_3)$, branching ratio as for $CH_3OOH$ + OH

A41020b_a01: $HOCHOOHO_2$ is assumed to directly decompose into CHOOOH and $HO_2$

A41021_a01: $HO_2$ elimination

A41022_a01: $k(HO_2+HO_2)$

A41023_a01: $k(HO_2+O_2^-)$

A41030_a01: $HO_2$ elimination

A42000a_a01: $CH_3CHOHO_2$ is assumed to directly decompose into $CH_3CHO$ + $HO_2$

A42001a_a01: $CH_3CHOHO_2$ is assumed to directly decompose into $CH_3CHO$ + $HO_2$

A42003_a01: $k(HO_2+O_2^-)$

A42004_a01: $k(HO_2+HO_2)$

A42005_a01: $k$ approximated from ($k(CH_3OOH+OH)$ /$k(CH_3OH+OH)$)

A42006_a01: $CH_2OHCHOHO_2$ is assumed to directly decompose into $HOCH_2CHO$ + $HO_2$

A42007_a01: $CH_2OHCHOHO_2$ is assumed to directly decompose into $HOCH_2CHO$ + $HO_2$

A42010_a01: $k$ based on Monod et al. (2005): $k$=$k$(2 $CH_3CH_2(OO)$)

A42014_a01: $HO_2$ elimination

A42016a_a01: $k$ assumed to be the same as for $CH_3CHO$ + $NO_3$

A42016b_a01: See branch a.

A42017_a01: $k(CH_3CHOHOH+O_2^-)$

A42018_a01: $HO_2$ elimination

A42019_a01: $k$ based on von Sonntag (1987)

A42020_a01: $k$ based on von Sonntag (1987)

A42022a_a01: $k(CH_3CHOHOH+NO_3)$

A42022b_a01: See branch a.

A42022c_a01: See branch a.

A42023b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + $HO_2$

A42024a_a01: $k$ based on Neta and Huie (1986)

A42024b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + $HO_2$

A42025_a01: $HO_2$ elimination

A42030b_a01: $CH_3CHOOHO_2$ is assumed to directly decompose into $CH_3CO_2H$ and $HO_2$

A42031b_a01: $CH_3CHOHO_2$ is assumed to directly decompose into $CH_3CHO + HO_2$

A42032_a01: $k(HO_2+O_2^-)$

A42033_a01: $k(HO_2+HO_2)$

A42034_a01: $k(HO_2+HO_2)$

A42035_a01: $k(HO_2+O_2^-)$

A42037_a01: $k(HO_2+HO_2)$

A42038_a01: $k(HO_2+O_2^-)$

A42144a_a01: $k$ assumed to be the same as $C_2H_5OOH$ + OH based on Monod et al. (2007)

A42144b_a01: See branch a.

A42146a_a01: $k$ assumed to be the same as $C_2H_5OOH$ + OH based on Monod et al. (2007)

A42146b_a01: See branch a.

A42148_a01: $HO_2$ elimination

A42149_a01: $HO_2$ elimination

A42150a_a01: COOHOO is not formed but directly dissociates into $CO_2$ + $HO_2$. Rate coefficient based on Buxton et al. (1988)

A42150b_a01: See branch a.

A42151a_a01: COOHOO is not formed but directly dissociates into $CO_2$ + $HO_2$. Rate coefficient based on Gaillard de Sémainville et al. (2007)

A42151b_a01: See branch a.

A42156b_a01: COOHOO is not formed but directly dissociates into $CO_2$ + $HO_2$.

A42157a_a01: $k(CHOHOHCHOHOH+NO_3)$

A42157b_a01: COOHOO is not formed but directly dissociates into $CO_2$ + $HO_2$

A42161_a01: $HO_2$ elimination

A42162_a01: $HO_2$ elimination

A42163a_a01: $k(HOCH_2CHO\ +OH)$

A42163b_a01: See branch a.

A42164a_a01: $k(HOCH_2CHO+NO_3)$

A42164b_a01: See branch a.

A42165a_a01: $k(HOCH_2CHOHOH+OH)$

A42165b_a01: See branch a.

A42165c_a01: See branch a.

A42166a_a01: $k(HOCH_2CHOHOH+NO_3)$

A42166b_a01: See branch a.

A42166c_a01: See branch a.

A42167_a01: pH-dependent

A42169_a01: $k = 2 \times k(HOCH_2OH+OH)$

A42471_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

A42472_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

A42473_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

A43000a_a01: Intermidate reaction with $O_2^-$ and $CH(OH)_2COCH_2O_2$ neglected

A43001_a01: $CH(OH)_2COCH_2O_2$ neglected

A43002_a01: $CO_2$ added for mass balance intermediate reactions neglected

A43004_a01: $CO_2$ added for mass balance intermediate reactions neglected

A43010a_a01: $CH_2(OH)COCH_2O_2$ was negected with a branching ratio 0.16 added to $CH_3COCHOHO_2$

A43013_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Monod et al., 2005)

A43014_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Herrmann et al., 1994)

A43015a_a01: $k$ calculated comparing the rates $(CH_3OH + OH/CH_3OOH + OH)$ and $(ACETOL + OH/HYPERACET + OH)$

A43015b_a01: $k$ from $CH_3OOH + OH \rightarrow HCHO$.

A43016_a01: $k$ taked from the reaction of the hydrated form of MGLYOX and $NO_3$

A43017_a01: $k$ from $CH_3O_2 + HO_2$

A43018_a01: $k$ from $CH_3O_2 + O_2^-$

A43019a_a01: $k$ calculated comparing $CH_3OH + OH$ / $CH_3OOH + OH$ with $IPROPL + OH$

A43019b_a01: $k$ calculated comparing $CH3OH + OH$ / $CH3OOH + OH$ with $ACETOL + OH$ / $HYPERCET + OH$

A43020_a01: $k$ taken from the reaction of the hydrated form of MGLYOX and $NO_3$

A43021_a01: $k$ from $CH_3O_2 + HO_2$

A43022_a01: $k$ from $CH_3O_2 + O_2^-$

A43023_a01: pH-dependent

A43025_a01: $k = 2 \times k(HOCH_2OH+OH)$

A44010_a01: $k = 2 \times k(CHOHOHCHOHOH+OH)$

A44011_a01: $k = 2 \times k(CHOHOHCHOHOH+OH)$

A44012_a01: $k = 2 \times k(CHOHOHCHOHOH+OH)$

A46000_a01: Assumed to be the same as for glyoxal

A46001_a01: Assumed to be the same as for glyoxal

A46002_a01: $k = 2 \times k(CH_3COCHOHOH+OH)$

A46003_a01: Assumed to be the same as for glyoxal

A46004_a01: Assumed to be the same as for glyoxal

A46005_a01: $k = 2 \times k(CH_3COCHOHOH+OH)$

A61002_a01: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A63001_a01: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A64000_a01: $k$ taken from $H_2O_2$+$Cl_2^-$ (Yu, 2004).

A74000_a01: Assumed to be the same as for $Br_2^-$ + $H_2O_2$.

A76003_a01: The rate coefficient is defined as backward reaction divided by equilibrium constant.

A91005_a01: The rate coefficient for the sum of the paths (leading to either $HSO_5^-$ or $SO_4^{2-}$) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A91006_a01: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of $SO_4^-$, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, $SO_4^{2-}$ is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.

A92005_a01: D. Sedlak, pers. comm. (1993).

A92008_a01: D. Sedlak, pers. comm. (1993).

A94100_a01: $2.48 \times 10^7 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.

A94102_a01: $790 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.

A94108a_a01: $k(H_2O_2+SO_4^-)$, branching ratio as for $CH_3OOH$ + OH

A94108b_a01: See branch a.

A94200_a01: $k(CH_3OO+HSO_3^-)$

A94201_a01: $k(CH_3OO+HSO_3^-)$

A94202a_a01: $CH_3CHOHO_2$ is assumed to directly decompose into $CH_3CHO$ + $HO_2$

A94203b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + $HO_2$

A96005_a01: Assumed to be the same as for $SO_3^{2-}$ + HOCl.

A97005_a01: Assumed to be the same as for $SO_3^{2-}$ + HOBr.

A116005_a01: products assumed

A119001_a01: products assumed

A119002_a01: products assumed

A119004_a01: Assumed. Note that CAPRAM 2.4 lists $k$=4.3E7 from Herrmann Air Pollution Research Report 57 and it also lists $k$= 2.65E7 from Williams PhD 1996 http://lib.leeds.ac.uk/record=b1835184~S5. Brand and van Eldik (1995) also list $k$=3.56E4 from Waygood EUROTRAC 1992 report.

A119006_a01: 3E8*6500/(48000+6500)

A119008_a01: Assuming that the intermediate $S_2O_6^{2-}$ dissociates quickly.

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