

The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs7

MECCA version: 3.8b

Date: December 18, 2017.

Selected reactions:

“Tr && G && !Cl && !Br && !I && !Hg”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 2664

Aqueous phase: 0

All species: 2664

Number of reactions in selected mechanism:

Gas phase (Gmn): 1670

Aqueous phase (Amn): 0

Henry (Hmn): 0

Photolysis (Jmn): 324

Aqueous phase photolysis (PHmn): 0

Heterogeneous (HETmn): 0

Equilibria (EQmn): 0

Isotope exchange (IEXmn): 0

Tagging equations (TAGmn): 0

Dummy (Dmn): 0

All equations: 1994

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Evidence from the Modelling of HOx Measurements over Cyprus”

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<https://www.atmospheric-chemistry-and-physics.net>

Table 1: Gas phase reactions

| # | labels | reaction | rate coefficient | reference |
|-------|----------|---|--|---|
| G1000 | UpStTrG | $O_2 + O(^1D) \rightarrow O(^3P) + O_2$ | $3.3E-11*EXP(55./temp)$ | Sander et al. (2011) |
| G1001 | UpStTrG | $O_2 + O(^3P) \rightarrow O_3$ | $6.E-34*((temp/300.)**(-2.4))*cair$ | Sander et al. (2011) |
| G2100 | UpStTrG | $H + O_2 \rightarrow HO_2$ | $k_3rd(temp, cair, 4.4E-32, 1.3, 7.5E-11, -0.2, 0.6)$ | Sander et al. (2011) |
| G2104 | UpStTrG | $OH + O_3 \rightarrow HO_2 + O_2$ | $1.7E-12*EXP(-940./temp)$ | Sander et al. (2011) |
| G2105 | UpStTrG | $OH + H_2 \rightarrow H_2O + H$ | $2.8E-12*EXP(-1800./temp)$ | Sander et al. (2011) |
| G2107 | UpStTrG | $HO_2 + O_3 \rightarrow OH + 2 O_2$ | $1.E-14*EXP(-490./temp)$ | Sander et al. (2011) |
| G2109 | UpStTrG | $HO_2 + OH \rightarrow H_2O + O_2$ | $4.8E-11*EXP(250./temp)$ | Sander et al. (2011) |
| G2110 | UpStTrG | $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$ | k_HO2_HO2 | Christensen et al. (2002), Kircher and Sander (1984)* |
| G2111 | UpStTrG | $H_2O + O(^1D) \rightarrow 2 OH$ | $1.63E-10*EXP(60./temp)$ | Sander et al. (2011) |
| G2112 | UpStTrG | $H_2O_2 + OH \rightarrow H_2O + HO_2$ | $1.8E-12$ | Sander et al. (2011) |
| 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* |
| G3101 | UpStTrGN | $N_2 + O(^1D) \rightarrow O(^3P) + N_2$ | $2.15E-11*EXP(110./temp)$ | Sander et al. (2011) |
| G3103 | UpStTrGN | $NO + O_3 \rightarrow NO_2 + O_2$ | $3.E-12*EXP(-1500./temp)$ | Sander et al. (2011) |
| G3106 | StTrGN | $NO_2 + O_3 \rightarrow NO_3 + O_2$ | $1.2E-13*EXP(-2450./temp)$ | Sander et al. (2011) |
| G3108 | StTrGN | $NO_3 + NO \rightarrow 2 NO_2$ | $1.5E-11*EXP(170./temp)$ | Sander et al. (2011) |
| G3109 | UpStTrGN | $NO_3 + NO_2 \rightarrow N_2O_5$ | k_NO3_NO2 | Sander et al. (2011)* |
| G3110 | StTrGN | $N_2O_5 \rightarrow NO_2 + NO_3$ | $k_NO3_NO2/(2.7E-27*EXP(11000./temp))$ | Sander et al. (2011)* |
| G3200 | TrGN | $NO + OH \rightarrow HONO$ | $k_3rd(temp, cair, 7.0E-31, 2.6, 3.6E-11, 0.1, 0.6)$ | Sander et al. (2011) |
| G3201 | UpStTrGN | $NO + HO_2 \rightarrow NO_2 + OH$ | $3.3E-12*EXP(270./temp)$ | Sander et al. (2011) |
| G3202 | UpStTrGN | $NO_2 + OH \rightarrow HNO_3$ | $k_3rd(temp, cair, 1.8E-30, 3.0, 2.8E-11, 0., 0.6)$ | Sander et al. (2011) |
| G3203 | StTrGN | $NO_2 + HO_2 \rightarrow HNO_4$ | k_NO2_HO2 | Sander et al. (2011)* |
| G3204 | TrGN | $NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$ | $3.5E-12$ | Sander et al. (2011) |
| G3205 | TrGN | $HONO + OH \rightarrow NO_2 + H_2O$ | $1.8E-11*EXP(-390./temp)$ | Sander et al. (2011) |
| G3206 | StTrGN | $HNO_3 + OH \rightarrow H_2O + NO_3$ | k_HNO3_OH | Sander et al. (2011)* |
| G3207 | StTrGN | $HNO_4 \rightarrow NO_2 + HO_2$ | $k_NO2_HO2/(2.1E-27*EXP(10900./temp))$ | Sander et al. (2011)* |
| G3208 | StTrGN | $HNO_4 + OH \rightarrow NO_2 + H_2O$ | $1.3E-12*EXP(380./temp)$ | Sander et al. (2011) |

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

| # | labels | reaction | rate coefficient | reference |
|--------|--------|---|--|--|
| G3209 | TrGN | $\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$ | $1.7\text{E-}12 \cdot \text{EXP}(-710./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3210 | TrGN | $\text{NH}_2 + \text{O}_3 \rightarrow \text{NH}_2\text{O} + \text{O}_2$ | $4.3\text{E-}12 \cdot \text{EXP}(-930./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3211 | TrGN | $\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$ | $4.8\text{E-}07 \cdot \text{EXP}(-628./\text{temp})$ $\cdot \text{temp}^{**}(-1.32)$ | Kohlmann and Poppe (1999) |
| G3212 | TrGN | $\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$ | $9.4\text{E-}09 \cdot \text{EXP}(-356./\text{temp})$ $\cdot \text{temp}^{**}(-1.12)$ | Kohlmann and Poppe (1999) |
| G3213 | TrGN | $\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$ | $1.92\text{E-}12 \cdot ((\text{temp}/298.)^{**}(-1.5))$ | Kohlmann and Poppe (1999) |
| G3214 | TrGN | $\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$ | $1.41\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-1.5))$ | Kohlmann and Poppe (1999) |
| G3215 | TrGN | $\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$ | $1.2\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-2.0))$ | Kohlmann and Poppe (1999) |
| G3216 | TrGN | $\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$ | $0.8\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-2.0))$ | Kohlmann and Poppe (1999) |
| G3217 | TrGN | $\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{NH}_2 + \text{O}_2$ | $1.2\text{E-}14$ | Kohlmann and Poppe (1999) |
| G3218 | TrGN | $\text{NH}_2\text{O} \rightarrow \text{NHOH}$ | $1.3\text{E}3$ | Kohlmann and Poppe (1999) |
| G3219 | TrGN | $\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$ | $8.0\text{E-}11 \cdot \text{EXP}(-500./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3220 | TrGN | $\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$ | $1.66\text{E-}12 \cdot \text{EXP}(-1500./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3221 | TrGN | $\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$ | $1.0\text{E-}12 \cdot \text{EXP}(-1000./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3222 | TrGN | $\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$ | $1.66\text{E-}12$ | Kohlmann and Poppe (1999) |
| G3223 | TrGN | $\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$ | $4.13\text{E-}11 \cdot \text{EXP}(-2138./\text{temp})$ | Kohlmann and Poppe (1999) |
| G3224 | TrGN | $\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$ | $3.65\text{E-}14 \cdot \text{EXP}(-4600./\text{temp})$ | Kohlmann and Poppe (1999) |
| G4101 | StTrG | $\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$ | $1.85\text{E-}20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp})$ $-987./\text{temp})$ | Atkinson (2003) |
| G4102 | TrG | $\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{HCHO} + .85 \text{HO}_2 + .15 \text{CH}_3\text{O} + \text{H}_2\text{O}$ | $6.38\text{E-}18 \cdot \text{temp}^{**}2 \cdot \text{EXP}(144./\text{temp})$ | Atkinson et al. (2006) |
| G4103a | StTrG | $\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$ | $3.8\text{E-}13 \cdot \text{EXP}(780./\text{temp}) / (1.+1./$ $498. \cdot \text{EXP}(1160./\text{temp}))$ | Atkinson et al. (2006) |
| G4103b | StTrG | $\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$ | $3.8\text{E-}13 \cdot \text{EXP}(780./\text{temp}) / (1.+$ $498. \cdot \text{EXP}(-1160./\text{temp}))$ | Atkinson et al. (2006) |
| G4104a | StTrGN | $\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$ | $2.3\text{E-}12 \cdot \text{EXP}(360./\text{temp}) \cdot (1.-\text{beta}_$ $\text{CH3NO3})$ | Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998) |
| G4104b | StTrGN | $\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$ | $2.3\text{E-}12 \cdot \text{EXP}(360./\text{temp}) \cdot \text{beta}_$ CH3NO3 | Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)* |
| G4105 | TrGN | $\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$ | $1.2\text{E-}12$ | Atkinson et al. (2006) |
| G4106a | StTrG | $\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{O}_2$ | $7.4\text{E-}13 \cdot \text{EXP}(-520./\text{temp}) \cdot \text{R02} \cdot 2.$ | Atkinson et al. (2006) |

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

| # | labels | reaction | rate coefficient | reference |
|--------|---------|--|--|---------------------------|
| G4106b | StTrG | $\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$ | $(k_{\text{CH302}} - 7.4\text{E}-13 * \text{EXP}(-520./\text{temp})) * \text{R02} * 2.$ | Atkinson et al. (2006) |
| G4107 | StTrG | $\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{CH}_3\text{O}_2 + .4 \text{HCHO} + .4 \text{OH} + \text{H}_2\text{O}$ | $k_{\text{CH300H_OH}}$ | Wallington et al. |
| G4108 | StTrG | $\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$ | $9.52\text{E}-18 * \text{EXP}(2.03 * \text{LOG}(\text{temp}) + 636./\text{temp})$ | Sivakumaran et al. (2003) |
| G4109 | TrGN | $\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$ | $3.4\text{E}-13 * \text{EXP}(-1900./\text{temp})$ | Sander et al. (2011) |
| G4110 | UpStTrG | $\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$ | $(1.57\text{E}-13 + \text{cair} * 3.54\text{E}-33)$ | McCabe et al. (2001) |
| G4111 | TrG | $\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$ | $2.94\text{E}-14 * \text{exp}(786./\text{temp}) + 9.85\text{E}-13 * \text{EXP}(-1036./\text{temp})$ | Paulot et al. (2011) |
| G4114 | StTrGN | $\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$ | $k_{\text{NO2_CH302}}$ | Sander et al. (2011) |
| G4115 | StTrGN | $\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$ | $k_{\text{NO2_CH302}} / (9.5\text{E}-29 * \text{EXP}(11234./\text{temp}))$ | Sander et al. (2011) |
| G4116 | StTrGN | $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$ | $3.00\text{E}-14$ | see note* |
| G4117 | StTrGN | $\text{CH}_3\text{ONO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}_2$ | $4.0\text{E}-13 * \text{EXP}(-845./\text{temp})$ | Atkinson et al. (2006) |
| G4118 | StTrG | $\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$ | $1.3\text{E}-14 * \text{exp}(-663./\text{temp}) * c(\text{ind_02})$ | Chai et al. (2014) |
| G4119a | StTrGN | $\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$ | $k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 8.1\text{E}-29, 4.5, 2.1\text{E}-11, 0., 0.44)$ | Atkinson et al. (2006) |
| G4119b | StTrGN | $\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$ | $9.6\text{E}-12 * \text{EXP}(-1150./\text{temp})$ | Atkinson et al. (2006) |
| G4120a | StTrGN | $\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$ | $k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 2.6\text{E}-29, 2.8, 3.3\text{E}-11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/900.), \text{SP}))$ | Atkinson et al. (2006) |
| G4120b | StTrGN | $\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$ | $2.3\text{E}-12 * (\text{temp}/300.) ** 0.7$ | Atkinson et al. (2006) |
| G4121 | StTrG | $\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$ | $2.9\text{E}-16 * \text{exp}(-1000./\text{temp})$ | Sander et al. (2011) |
| G4122 | StTrGN | $\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$ | $1.\text{E}-10 * \text{exp}(-1764./\text{temp})$ | Nielsen et al. (1991) |
| G4123 | StTrG | $\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$ | $9.7\text{E}-15 * \text{EXP}(625./\text{temp})$ | Atkinson et al. (2006) |
| G4124 | StTrG | $\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$ | $2.4\text{E}12 * \text{EXP}(-7000./\text{temp})$ | Atkinson et al. (2006) |
| G4125 | StTrG | $\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2 \text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$ | $5.6\text{E}-15 * \text{EXP}(2300./\text{temp})$ | Atkinson et al. (2006) |
| G4126 | StTrGN | $\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$ | $0.7275 * 2.3\text{E}-12 * \text{EXP}(360./\text{temp})$ | Atkinson et al. (2006)* |
| G4127 | StTrGN | $\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$ | $1.2\text{E}-12$ | see note* |
| G4129a | StTrG | $\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$ | $(k_{\text{CH302}} * 5.5\text{E}-12) ** 0.5 * \text{R02} * 2.$ | Atkinson et al. (2006) |
| G4129b | StTrG | $\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$ | $(k_{\text{CH302}} * 5.7\text{E}-14 * \text{EXP}(750./\text{temp})) ** 0.5 * \text{R02} * 2.$ | Atkinson et al. (2006) |
| G4130a | StTrG | $\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$ | $0.6 * k_{\text{CH300H_OH}}$ | Taraborrelli (2010)* |
| G4130b | StTrG | $\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$ | $k_{\text{rohro}} + k_{\text{s*f_sooh*f_soh}}$ | Taraborrelli (2010)* |

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

| # | labels | reaction | rate coefficient | reference |
|-------|--------|--|---|---|
| G4132 | StTrG | $\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$ | $k_{\text{rohro}} + 2 \cdot k_{\text{s*f_soh*f_soh}}$ | Taraborrelli (2010)* |
| G4133 | StTrG | $\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$ | 1.4E-10 | Bossolasco et al. (2014)* |
| G4134 | StTrG | $\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$ | $1.124\text{E}+14 \cdot \text{EXP}(-10000/\text{temp})$ | see note* |
| G4135 | StTrG | $\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$ | $k_{\text{CH200_N02}} \cdot 3.6\text{E}-6$ | Ouyang et al. (2013)* |
| G4136 | StTrG | $\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$ | 5.2E-12 | Chao et al. (2015), Lewis et al. (2015)* |
| G4137 | StTrGN | $\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$ | 6.E-14 | Welz et al. (2012)* |
| G4138 | StTrGN | $\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$ | $k_{\text{CH200_N02}}$ | Welz et al. (2012), Stone et al. (2014)* |
| G4140 | StTrG | $\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$ | 3.6E-14 | Vereecken et al. (2012) |
| G4141 | StTrG | $\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$ | 1.E-10 | Welz et al. (2014)* |
| G4142 | StTrG | $\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$ | 1.7E-12 | Stone et al. (2014)* |
| G4143 | StTrG | $\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$ | 5.E-12 | Vereecken et al. (2012)* |
| G4144 | StTrG | $\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$ | 5.E-12 | Vereecken et al. (2012)* |
| G4145 | StTrG | $\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$ | 5.E-12 | Vereecken et al. (2012) |
| G4146 | StTrG | $\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$ | 1.E-12 | Vereecken et al. (2014) |
| G4147 | StTrG | $\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$ | 6.E-11 | Buras et al. (2014) |
| G4148 | StTrGN | $\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$ | $k_{\text{N02_CH302}}$ | Sander et al. (2011) |
| G4149 | StTrGN | $\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$ | $k_{\text{N02_CH302}} / (9.5\text{E}-29 \cdot \text{EXP}(11234./\text{temp}))$ | Sander et al. (2011), Barnes et al. (1985)* |
| G4150 | StTrGN | $\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$ | $9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp}) \cdot f_{\text{soh}}$ | see note* |
| G4151 | StTrG | $\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$ | $k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 7.0\text{E}-31, 3., 1.8\text{E}-12, -1.1, 0.33)$ | Atkinson et al. (2006) |
| G4152 | StTrG | $\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{HCHO} + .956 \text{H} + .044 \text{CH}_3\text{O} + \text{O}_2$ | $5.1\text{E}-12 \cdot \text{exp}(-210./\text{temp})$ | Albaladejo et al. (2002), Ogryzlo et al. (1981) |
| G4153 | StTrG | $\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{HCHO} + .83 \text{H} + .17 \text{CO} + .17 \text{H}_2 + .17 \text{H}$ | 1.3E-10 | Atkinson et al. (2006) |
| G4154 | StTrG | $\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$ | 2.53E-14 | Albaladejo et al. (2002)* |
| G4155 | StTrG | $\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{CH}_3 + .75 \text{O}_2 + .25 \text{HCHO} + .25 \text{OH}$ | 2.5E-11 | Baulch et al. (2005) |
| G4156 | StTrG | $\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$ | 4.3E-11 | Zellner et al. (1988) |
| G4157 | StTrG | $\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{OH} + .7 \text{CO} + .3 \text{H} + .3 \text{CO}_2 + \text{HO}_2$ | $3.\text{E}-11 \cdot \text{EXP}(-1600./\text{temp})$ | Sander et al. (2011) |
| G4158 | TrG | $\text{CH}_2\text{OO}^* \rightarrow .37 \text{CH}_2\text{OO} + .47 \text{CO} + .47 \text{H}_2\text{O} + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH}$ | KDEC | Atkinson et al. (2006) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|---|---|
| G4159 | TrGN | $\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$ | $k_{3rd}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$ | Kleinböhl et al. (2006) |
| G4160a | TrGN | $\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{HCN}$ | $1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.15 * \text{EXP}(200/\text{temp})$ | Strekowski et al. (2010) |
| G4160b | TrGN | $\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{NCO}$ | $1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.68/2.$ | Strekowski et al. (2010)* |
| G4160c | TrGN | $\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{CN}$ | $1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * (1. - (0.68/2. + 0.15 * \text{EXP}(200/\text{temp})))$ | Strekowski et al. (2010)* |
| G4161 | TrGN | $\text{HCN} + \text{O}(^3\text{P}) \rightarrow \text{H} + \text{NCO}$ | $1.0\text{E-}11 * \text{EXP}(-4000./\text{temp})$ | Sander et al. (2011)* |
| G4162 | TrGN | $\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}(^3\text{P})$ | $1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.75$ | Baulch et al. (2005) |
| G4163 | TrGN | $\text{CN} + \text{O}_2 \rightarrow \text{CO} + \text{NO}$ | $1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.25$ | Baulch et al. (2005) |
| G4164 | TrGN | $\text{NCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{NO}$ | $7.\text{E-}15$ | Becker et al. (2000)* |
| G42000 | TrGC | $\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$ | $1.49\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(-499./\text{temp})$ | Atkinson et al. (2006) |
| G42001 | TrGC | $\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{OO}^*$ | $9.1\text{E-}15 * \text{EXP}(-2580./\text{temp})$ | Atkinson et al. (2006)* |
| G42002 | TrGC | $\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$ | $k_{3rd_iupac}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$ | Atkinson et al. (2006), Rickard and Pascoe (2009) |
| G42003 | TrGC | $\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$ | $7.5\text{E-}13 * \text{EXP}(700./\text{temp})$ | Sander et al. (2011) |
| G42004a | TrGCN | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$ | $2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * (1. - \text{beta_C2H5N03})$ | Atkinson et al. (2006), Butkovskaya et al. (2010) |
| G42004b | TrGCN | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$ | $2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * \text{beta_C2H5N03}$ | Atkinson et al. (2006), Butkovskaya et al. (2010) |
| G42005 | TrGCN | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$ | $2.3\text{E-}12$ | Wallington et al. |
| G42006 | TrGC | $\text{C}_2\text{H}_5\text{O}_2 \rightarrow .8 \text{CH}_3\text{CHO} + .6 \text{HO}_2 + .2 \text{C}_2\text{H}_5\text{OH}$ | $2. * (7.6\text{E-}14 * k_{\text{CH302}}) * (.5) * \text{R02}$ | Taraborrelli (2016), Atkinson et al. (2006) |
| G42007a | TrGC | $\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$ | $0.6 * k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G42007b | TrGC | $\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{OH}$ | k_{s*f_sooh} | Taraborrelli (2016) |
| G42008a | TrGC | $\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O}$ | $4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.95$ | Atkinson et al. (2006) |
| G42008b | TrGC | $\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$ | $4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.05$ | Atkinson et al. (2006) |
| G42009 | TrGCN | $\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HNO}_3$ | KN03AL | Rickard and Pascoe (2009) |
| G42010 | TrGC | $\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$ | $4.0\text{E-}14 * \text{EXP}(850./\text{temp})$ | Atkinson et al. (2006)* |
| G42011a | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$ | $5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.61$ | Groß et al. (2014) |
| G42011b | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$ | $5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.23$ | Groß et al. (2014) |
| G42011c | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$ | $5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.16$ | Groß et al. (2014) |
| G42012 | TrGCN | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$ | $8.1\text{E-}12 * \text{EXP}(270./\text{temp})$ | Tyndall et al. (2001a) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|---|
| G42013 | TrGCN | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$ | k_CH3C03_NO2 | Sander et al. (2011)* |
| G42014 | TrGCN | $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$ | 4.E-12 | Canosa-Mas et al. (1996) |
| G42017a | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3 + \text{CO}_2$ | k1_R02RC03*0.9 | Taraborrelli (2016) |
| G42017b | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOH}$ | k1_R02RC03*0.1 | Taraborrelli (2016) |
| G42018 | TrGC | $\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$ | 0.6*k_CH300H_OH | Rickard and Pascoe (2009)* |
| G42020 | TrGCN | $\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$ | 3.00E-14 | Rickard and Pascoe (2009) |
| G42021 | TrGCN | $\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$ | k_PAN_M | Sander et al. (2011)* |
| G42022a | TrGC | $\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$ | k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, 2., 0.6)*.71 | Sander et al. (2011), Glowacki et al. (2012) |
| G42022b | TrGC | $\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$ | k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, 2., 0.6)*(1.-.71) | Sander et al. (2011), Glowacki et al. (2012) |
| G42023a | TrGC | $\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$ | 8.00E-12*0.80 | Atkinson et al. (2006) |
| G42023b | TrGC | $\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$ | 8.00E-12*0.20 | Atkinson et al. (2006) |
| G42024a | TrGC | $\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$ | 5.1E-12*(1.-1./(1+1.85E-18*cair)) | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42024b | TrGC | $\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$ | 5.1E-12*1./(1+1.85E-18*cair) | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42025 | TrGC | $\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$ | KDEC | Taraborrelli (2016) |
| G42026 | TrGCN | $\text{HOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{HNO}_3$ | KN03AL | Rickard and Pascoe (2009) |
| G42027a | TrGC | $\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$ | k1_R02RC03*0.9 | Taraborrelli (2016) |
| G42027b | TrGC | $\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$ | k1_R02RC03*0.1 | Taraborrelli (2016) |
| G42028a | TrGC | $\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$ | KAPH02*rco3_oh | Taraborrelli (2016), Groß et al. (2014) |
| G42028b | TrGC | $\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$ | KAPH02*rco3_ooh | Taraborrelli (2016), Groß et al. (2014) |
| G42028c | TrGC | $\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_2\text{H} + \text{O}_3$ | KAPH02*rco3_o3 | Taraborrelli (2016), Groß et al. (2014) |
| G42029 | TrGCN | $\text{HOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G42030 | TrGCN | $\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$ | k_CH3C03_NO2 | Rickard and Pascoe (2009) |
| G42031 | TrGCN | $\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$ | KR02N03*1.60 | Rickard and Pascoe (2009) |
| G42032 | TrGC | $\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{HCHO} + .09 \text{CO}_2 + .91 \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$ | k_co2h+k_sf_soh*sf_co2h | Taraborrelli (2016) |
| G42033a | TrGC | $\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$ | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G42033b | TrGC | $\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$ | k_sf_soh*sf_co2h | Taraborrelli (2016) |
| G42034 | TrGCN | $\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|---|
| G42035 | TrGCN | PHAN + OH → HCHO + CO + NO ₂ + H ₂ O | k_s*f_soh*f_cpan+k_rohro | Taraborrelli (2016) |
| G42036 | TrGC | GLYOX + OH → HCOCO + H ₂ O | 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 | KN03AL | Rickard and Pascoe (2009) |
| G42038a | TrGC | HCOCO → CO + CO + HO ₂ | 7.E11*EXP(-3160./temp) +5.E-12*c(ind_02) | Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009) |
| G42037b | TrGC | HCOCO → HCOCO ₃ | 5.E-12*c(ind_02)*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_02) *(1.-3.2*exp(-550./temp)) | Lockhart et al. (2013), Rickard and Pascoe (2009) |
| G42039a | TrGC | HCOCO ₃ → CO + HO ₂ + CO ₂ | k1_R02RC03*0.9 | Taraborrelli (2016) |
| G42039b | TrGC | HCOCO ₃ → HCOCO ₂ H | k1_R02RC03*0.1 | Taraborrelli (2016) |
| G42040 | TrGC | HCOCO ₃ + HO ₂ → HO ₂ + CO + CO ₂ + OH | KAPH02 | Feierabend et al. (2008), Taraborrelli (2016) |
| G42041 | TrGCN | HCOCO ₃ + NO → HO ₂ + CO + NO ₂ + CO ₂ | KAPNO | Rickard and Pascoe (2009) |
| G42042 | TrGCN | HCOCO ₃ + NO ₃ → HO ₂ + CO + NO ₂ + CO ₂ | KR02N03*1.60 | Rickard and Pascoe (2009) |
| G42043 | TrGCN | HCOCO ₃ + NO ₂ → HO ₂ + CO + NO ₃ + CO ₂ | k_CH3C03_N02 | Orlando and Tyndall (2001), Taraborrelli (2016) |
| G42044 | TrGC | HCOCO ₂ H + OH → CO + HO ₂ + CO ₂ + H ₂ O | k_co2h+k_t*f_o*f_co2h | Taraborrelli (2016) |
| G42045a | TrGC | HCOCO ₃ H + OH → HCOCO ₃ + H ₂ O | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G42045b | TrGC | HCOCO ₃ H + OH → CO + CO ₂ + H ₂ O + OH | k_t*f_o*f_co2h | Taraborrelli (2016) |
| G42046 | TrGC | HOCH ₂ CH ₂ O ₂ → .6 HOCH ₂ CH ₂ O + .2 HOCH ₂ CHO + .2 ETHGLY | 2.*(7.8E-14*EXP(1000./temp) *k_CH302)**(.5)*R02 | Atkinson et al. (2006), Rickard and Pascoe (2009) |
| G42047 | TrGCN | HOCH ₂ CH ₂ O ₂ + NO → .25 HO ₂ + .5 HCHO + .75 HOCH ₂ CH ₂ O + NO ₂ | KR02N0*(1.-alpha_AN(3,1,0,0,0, temp, cair)) | Rickard and Pascoe (2009)* |
| G42048 | TrGCN | HOCH ₂ CH ₂ O ₂ + NO → ETHOHNO3 | KR02N0*alpha_AN(3,1,0,0,0,temp, cair) | Taraborrelli (2016) |
| G42049a | TrGC | HOCH ₂ CH ₂ O ₂ + HO ₂ → HYETHO2H | 1.53E-13*EXP(1300./temp) *(1.-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G42049b | TrGC | HOCH ₂ CH ₂ O ₂ + HO ₂ → HOCH ₂ CH ₂ O + OH | 1.53E-13*EXP(1300./temp) *rchohch2o2_oh | Rickard and Pascoe (2009) |
| G42050 | TrGCN | ETHOHNO3 + OH → .93 NO ₃ CH ₂ CHO + .93 HO ₂ + .07 HOCH ₂ CHO + .07 NO ₂ + H ₂ O | k_s*(f_soh*f_ch2ono2+f_ono2*f_pch2oh)+k_rohro | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|---|
| G42051a | TrGC | $\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009)* |
| G42051b | TrGC | $\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$ | $k_{\text{s*f_sooh*f_pch2oh}}$ | Taraborrelli (2016) |
| G42051c | TrGC | $\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$ | $k_{\text{s*f_soh*f_pch2oh+k_rohro}}$ | Taraborrelli (2016) |
| G42052a | TrGC | $\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HOCH}_2\text{CHO}$ | $6.00\text{E-}14 \cdot \text{EXP}(-550./\text{temp})$ $\cdot \text{C}(\text{ind_02})$ | Rickard and Pascoe (2009) |
| G42052b | TrGC | $\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HCHO} + \text{HCHO}$ | $9.50\text{E}13 \cdot \text{EXP}(-5988./\text{temp})$ | Rickard and Pascoe (2009) |
| G42053 | TrGC | $\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$ | $2 \cdot k_{\text{s*f_soh*f_pch2oh}} + 2 \cdot k_{\text{rohro}}$ | Taraborrelli (2016) |
| G42054 | TrGC | $\text{HCOCH}_2\text{O}_2 \rightarrow .6 \text{ HCHO} + .6 \text{ CO} + .6 \text{ HO}_2 + .2 \text{ GLYOX}$ $+ .2 \text{ HOCH}_2\text{CHO}$ | $k1_{\text{R02p0R02}}$ | Taraborrelli (2016) |
| G42055a | TrGC | $\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CHO}$ | $\text{KR02H02}(2) \cdot r_{\text{coch2o2_ooh}}$ | Taraborrelli (2016) |
| G42055b | TrGC | $\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{OH}$ | $\text{KR02H02}(2) \cdot r_{\text{coch2o2_oh}}$ | Taraborrelli (2016) |
| G42056a | TrGCN | $\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$ | $\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair}))$ | Taraborrelli (2016) |
| G42056b | TrGCN | $\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$ | $\text{KR02N0} \cdot \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair})$ | Taraborrelli (2016) |
| G42057 | TrGCN | $\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G42058a | TrGC | $\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G42058b | TrGC | $\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH}$ | $.8 \cdot 8.\text{E-}12$ | Taraborrelli (2016)* |
| G42058c | TrGC | $\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$ | $k_{\text{s*f_sooh*f_cho}}$ | Taraborrelli (2016) |
| G42059 | TrGCN | $\text{HOOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HNO}_3$ | KN03AL | Rickard and Pascoe (2009) |
| G42060 | TrGCN | $\text{HOOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$ | KAPNO | Taraborrelli (2016) |
| G42061 | TrGCN | $\text{HOOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$ | $\text{KR02N03} \cdot 1.60$ | Taraborrelli (2016) |
| G42062a | TrGC | $\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 2 \text{ OH} + \text{HCHO} + \text{CO}_2$ | $\text{KAPH02} \cdot r_{\text{co3_oh}}$ | Taraborrelli (2016) |
| G42062b | TrGC | $\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$ | $\text{KAPH02} \cdot r_{\text{co3_ooh}}$ | Taraborrelli (2016) |
| G42062c | TrGC | $\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{O}_3$ | $\text{KAPH02} \cdot r_{\text{co3_o3}}$ | Taraborrelli (2016) |
| G42063a | TrGC | $\text{HOOCH}_2\text{CO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$ | $k1_{\text{R02RC03}} \cdot 0.9$ | Taraborrelli (2016) |
| G42063b | TrGC | $\text{HOOCH}_2\text{CO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$ | $k1_{\text{R02RC03}} \cdot 0.1$ | Taraborrelli (2016) |
| G42064a | TrGC | $\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{H}_2\text{O}$ | $2 \cdot 0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G42064b | TrGC | $\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{OH} + \text{H}_2\text{O}$ | $k_{\text{s*f_sooh*f_co2h}}$ | Taraborrelli (2016) |
| G42065 | TrGC | $\text{HOOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCO}_2\text{H} + \text{OH} + \text{H}_2\text{O}$ | $k_{\text{s*f_sooh*f_co2h+k_co2h}}$ | Taraborrelli (2016) |
| G42066 | TrGC | $\text{CH}_2\text{CO} + \text{OH} \rightarrow .6 \text{ HCHO} + .6 \text{ HO}_2 + .6 \text{ CO} + .4$ $\text{HOOCH}_2\text{CO}_2\text{H}$ | $2.8\text{E-}12 \cdot \text{exp}(510./\text{temp})$ | Baulch et al. (2005), Taraborrelli (2016) |
| G42067a | TrGC | $\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{OH}$ | $(k_{\text{t*f_tooh*f_toh}} + k_{\text{rohro}})$ | Taraborrelli (2016) |
| G42067b | TrGC | $\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|---------|--|---|---|
| G42068 | TrGC | $\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$ | $3.46\text{E}12 \cdot \text{EXP}(-12500./ (1.98 \cdot \text{temp}))$ | Hermans et al. (2005), Taraborrelli (2016) |
| G42069 | TrGC | $\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$ | $3.46\text{E}12 \cdot \text{EXP}(-12500./ (1.98 \cdot \text{temp})) / (6.34\text{E}26 \cdot \text{EXP}(-14700./ (1.98 \cdot \text{temp})))$ | Hermans et al. (2005), Taraborrelli (2016) |
| G42070 | TrGC | $\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{CH}_3\text{CHOHOOH} + .3 \text{CH}_3\text{COOH} + .2 \text{CH}_3 + .2 \text{HCOOH} + .2 \text{OH}$ | $5.6\text{E}-15 \cdot \text{EXP}(2300./ \text{temp})$ | Taraborrelli (2016) |
| G42071 | TrGC | $\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$ | k1_R02s0R02 | Taraborrelli (2016) |
| G42072 | TrGCN | $\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$ | KR02NO | Taraborrelli (2016) |
| G42073 | TrGCN | $\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$ | $6.7\text{E}-13 \cdot \text{EXP}(-395./ \text{temp})$ | Atkinson et al. (2006) |
| G42074a | TrGCN | $\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{NO}_2 + \text{H}_2\text{O}$ | k_s*f_ch2ono2*f_ch | Paulot et al. (2009a), Taraborrelli (2016)* |
| G42074b | TrGCN | $\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{H}_2\text{O}$ | k_t*f_o*f_ch2ono2*3. | Paulot et al. (2009a), Taraborrelli (2016)* |
| G42075 | TrGCN | $\text{NO}_3\text{CH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{OH}$ | KAPH02 | Rickard and Pascoe (2009)* |
| G42076 | TrGCN | $\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{NO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G42077 | TrGCN | $\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G42078 | TrGCN | $\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$ | k1_R02RC03 | Rickard and Pascoe (2009)* |
| G42079 | TrGCN | $\text{NO}_3\text{CH}_2\text{CHO} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G42080 | StTrGCN | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2\text{NO}_2$ | k_3rd_iupac(temp, cair, 1.3E-29, 6.2, 8.8E-12, 0.0, 0.31) | Atkinson et al. (2006) |
| G42081 | StTrGCN | $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$ | 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 | $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$ | $9.50\text{E}-13 \cdot \text{EXP}(-650./ \text{temp})$ | Taraborrelli (2016)* |
| G42083a | TrGC | $\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$ | $5.1\text{E}-12 \cdot (1. - 1./ (1. + 9.4\text{E}-18 \cdot \text{cair}))$ | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42083b | TrGC | $\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$ | $5.1\text{E}-12 \cdot 1./ (1. + 9.4\text{E}-18 \cdot \text{cair})$ | Atkinson et al. (2006), Beyersdorf et al. (2010)* |
| G42084 | TrGC | $\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{C}_2\text{H}_5\text{O}_2 + .95 \text{HO}_2 + .05 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$ | $3.0\text{E}-12 \cdot \text{EXP}(20./ \text{temp})$ | Taraborrelli (2016), Atkinson et al. (2006) |
| G42085a | TrGCN | $\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$ | $8.1\text{E}-13 \cdot \text{EXP}(-1080./ \text{temp}) \cdot 0.40$ | Atkinson et al. (2006), Tyndall et al. (2001b)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|---|
| G42085b | TrGCN | $\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$ | $8.1\text{E-}13*\text{EXP}(-1080./\text{temp})*(1.-0.40)$ | Atkinson et al. (2006), Tyndall et al. (2001b)* |
| G42086a | TrGCN | $\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$ | $2.54\text{E-}10*\text{EXP}(-24./\text{temp})$ $*0.0269*\text{EXP}(137./\text{temp})$ | Strekowski et al. (2010) |
| G42086b | TrGCN | $\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{H} + \text{CO} + \text{HCN}$ | $2.54\text{E-}10*\text{EXP}(-24./\text{temp})*0.16$ | Strekowski et al. (2010)* |
| G42086c | TrGCN | $\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{CH}_3 + .5 \text{NCO} + .5 \text{NCCH}_2\text{O}_2 + .5 \text{OH}$ | $2.54\text{E-}10*\text{EXP}(-24./\text{temp})*(1.-(0.16+$ $0.0269*\text{EXP}(137./\text{temp})))$ | Strekowski et al. (2010)* |
| G42087 | TrGCN | $\text{NCCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$ | KR02NO | see note* |
| G42088 | TrGCN | $\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$ | KR02HO2(2) | see note* |
| G42089a | TrGC | $\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{HCHO}$ | k_CH2CHOH_OH_HCOOH | Taraborrelli (2016), So et al. (2014)* |
| G42089b | TrGC | $\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2$ | k_CH2CHOH_OH_ALD | Taraborrelli (2016), So et al. (2014) |
| G42090 | TrGC | $\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$ | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G42091 | TrGC | $\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$ | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G43000a | TrGC | $\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$ | k_s | Taraborrelli (2016) |
| G43000b | TrGC | $\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$ | 2.*k_p | Taraborrelli (2016) |
| G43001a | TrGC | $\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{CHOHO}_2 + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$ | $5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.57$ | Atkinson et al. (2006)* |
| G43001b | TrGC | $\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{OO}^*$ | $5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.43$ | Atkinson et al. (2006)* |
| G43002 | TrGC | $\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO}_2$ | 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 | $\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO}_3\text{BO}_2$ | $4.6\text{E-}13*\text{EXP}(-1155./\text{temp})$ | Wallington et al. |
| G43004 | TrGC | $\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$ | $1.9\text{E-}13*\text{EXP}(1300./\text{temp})$ | Atkinson (1997)* |
| G43005a | TrGCN | $\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$ | $2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\text{alpha}_\text{AN}(3,2,0,0,0,\text{temp},\text{cair}))$ | Wallington et al. |
| G43005b | TrGCN | $\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{ONO}_2$ | $2.7\text{E-}12*\text{EXP}(360./\text{temp})*\text{alpha}_\text{AN}(3,2,0,0,0,\text{temp},\text{cair})$ | Wallington et al. |
| G43006 | TrGC | $\text{iC}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{CH}_3\text{COCH}_3 + .2 \text{IPROPOL} + .6 \text{HO}_2$ | $2.*(1.6\text{E-}12*\text{EXP}(-2200./\text{temp})*\text{k_CH302})*(.5)*\text{R02}$ | Rickard and Pascoe (2009), Atkinson et al. (2006) |
| G43007a | TrGC | $\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$ | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G43007b | TrGC | $\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{OH}$ | k_t*f_tooh | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|---|
| 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. |
| 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. |
| G43010 | TrGC | $C_3H_7O_2 \rightarrow .8 CH_3COCH_3 + .2 NPROPOL + .6 HO_2$ | $2.*(k_CH302*3.E-13)**(.5)*R02$ | 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 | $CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$ | $8.6E-13*EXP(700./temp)*rcoch2o2_ooh$ | Tyndall et al. (2001a), Taraborrelli (2016) |
| G43012b | TrGC | $CH_3COCH_2O_2 + HO_2 \rightarrow OH + CH_3C(O) + HCHO$ | $8.6E-13*EXP(700./temp)*rcoch2o2_oh$ | Tyndall et al. (2001a), Taraborrelli (2016) |
| G43013a | TrGCN | $CH_3COCH_2O_2 + NO \rightarrow CH_3C(O) + HCHO + NO_2$ | $2.9E-12*EXP(300./temp)*(1.-alpha_AN(4,1,1,0,0,temp,cair))$ | Sander et al. (2011) |
| G43013b | TrGCN | $CH_3COCH_2O_2 + NO \rightarrow NOA$ | $2.9E-12*EXP(300./temp)*alpha_AN(4,1,1,0,0,temp,cair)$ | Sander et al. (2011) |
| G43014 | TrGC | $CH_3COCH_2O_2 \rightarrow .3 CH_3C(O) + .3 HCHO + .5 MGLYOX + .2 CH_3COCH_2OH$ | $k1_R02p0R02$ | Orlando and Tyndall (2012) |
| G43015a | TrGC | $CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2 + H_2O$ | $0.6*k_CH300H_OH$ | see note* |
| G43015b | TrGC | $CH_3COCH_2O_2H + OH \rightarrow MGLYOX + OH + H_2O$ | $k_s*f_sooh*f_co$ | Taraborrelli (2016) |
| 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. |
| G43021 | TrGCN | $CH_3COCH_2O_2 + NO_3 \rightarrow CH_3C(O) + HCHO + NO_2$ | $KR02N03$ | Rickard and Pascoe (2009) |
| G43022 | TrGC | $HYPPO2 \rightarrow CH_3CHO + HCHO + HO_2$ | $k1_R02s0R02$ | Rickard and Pascoe (2009) |
| G43023a | TrGC | $HYPPO2 + HO_2 \rightarrow HYPPO2H$ | $KR02H02(3)*(1.-rchohch2o2_oh)$ | Rickard and Pascoe (2009) |
| G43023b | TrGC | $HYPPO2 + HO_2 \rightarrow CH_3CHO + HCHO + HO_2 + OH$ | $KR02H02(3)*rchohch2o2_oh$ | Rickard and Pascoe (2009) |
| G43024a | TrGCN | $HYPPO2 + NO \rightarrow CH_3CHO + HCHO + HO_2 + NO_2$ | $KR02N0*(1.-alpha_AN(4,1,0,0,0,temp,cair))$ | Rickard and Pascoe (2009) |
| G43024b | TrGCN | $HYPPO2 + NO \rightarrow PROPOLNO3$ | $KR02N0*alpha_AN(4,1,0,0,0,temp,cair)$ | Rickard and Pascoe (2009) |
| G43025 | TrGCN | $HYPPO2 + NO_3 \rightarrow CH_3CHO + HCHO + HO_2 + NO_2$ | $KR02N03$ | Rickard and Pascoe (2009) |
| G43026a | TrGC | $HYPPO2H + OH \rightarrow HYPPO2$ | $0.6*k_CH300H_OH$ | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|---|--|
| G43026b | TrGC | $\text{HYPROPO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$ | $(k_{s*f_{soh*f_{pch2oh}+k_{t*f_{tooh*f_{pch2oh}}})}$ | Taraborrelli (2016) |
| G43027 | TrGCN | $\text{PRONO3BO2} + \text{HO}_2 \rightarrow \text{PR2O2HNO3}$ | KR02H02(3) | Rickard and Pascoe (2009) |
| G43028 | TrGCN | $\text{PRONO3BO2} + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G43029 | TrGCN | $\text{PRONO3BO2} + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$ | KR02N03 | Rickard and Pascoe (2009) |
| G43030a | TrGCN | $\text{PR2O2HNO3} + \text{OH} \rightarrow \text{PRONO3BO2}$ | $0.6*k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009) |
| G43030b | TrGCN | $\text{PR2O2HNO3} + \text{OH} \rightarrow \text{NOA} + \text{OH}$ | $k_{t*f_{tooh*f_{ch2ono2}}}$ | Taraborrelli (2016) |
| G43031 | TrGCN | $\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{HNO}_3$ | KN03AL*2.4 | Rickard and Pascoe (2009) |
| G43032 | TrGCN | $\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$ | $(k_{s*f_{co*f_{ono2}+k_{p*f_{co}}})}$ | Taraborrelli (2016) |
| G43033 | TrGC | $\text{HOCH}_2\text{COCHO} + \text{OH} \rightarrow .8609 \text{HOCH}_2\text{CO} + .8609 \text{CO} + .1391 \text{HCOCOCHO} + .1391 \text{HO}_2$ | $(1.9\text{E-}12*\text{EXP}(575./\text{temp})+k_{s*f_{soh*f_{co}}})}$ | Taraborrelli (2016) |
| G43034 | TrGCN | $\text{HOCH}_2\text{COCHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HNO}_3$ | KN03AL*2.4 | Taraborrelli (2016) |
| G43035 | TrGC | $\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{H}_2\text{O} + \text{CO}_2$ | $4.9\text{E-}14*\text{EXP}(276./\text{temp})}$ | Mellouki and Mu (2003), Taraborrelli (2016) |
| G43036 | TrGC | $\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{HCOCO} + .6 \text{HCHO} + .2 \text{HCOCOCHO} + .2 \text{HOCH}_2\text{COCHO}$ | $k1_{\text{R02p0R02}}$ | Taraborrelli (2016) |
| G43037 | TrGCN | $\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G43038a | TrGC | $\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$ | $\text{KR02H02(3)*rcoch2o2_ooh}$ | Taraborrelli (2016) |
| G43038b | TrGC | $\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$ | $\text{KR02H02(3)*rcoch2o2_oh}$ | Taraborrelli (2016) |
| G43039 | TrGCN | $\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G43040a | TrGC | $\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$ | $k_{t*f_{co*f_o}}$ | Taraborrelli (2016)* |
| G43040b | TrGC | $\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$ | $k_{s*f_{sooh*f_{co}}}$ | Taraborrelli (2016)* |
| G43040c | TrGC | $\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$ | $0.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G43041 | TrGCN | $\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$ | KN03AL*2.4 | Taraborrelli (2016) |
| G43042 | TrGC | $\text{HOCH}_2\text{COCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO}$ | $k1_{\text{R02p0R02}}$ | Taraborrelli (2016) |
| G43043a | TrGC | $\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$ | $\text{KR02H02(3)*rcoch2o2_ooh}$ | Taraborrelli (2016) |
| G43043b | TrGC | $\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{OH}$ | $\text{KR02H02(3)*rcoch2o2_oh}$ | Taraborrelli (2016) |
| G43044 | TrGCN | $\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G43045a | TrGC | $\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCHO} + \text{OH}$ | $k_{s*f_{sooh*f_{co}}}$ | Taraborrelli (2016) |
| G43045b | TrGC | $\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{O}_2$ | $.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G43045c | TrGC | $\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$ | $1.60\text{E-}12*\text{EXP}(305./\text{temp})}$ | Taraborrelli (2016)* |
| G43046 | TrGC | $\text{CH}_3\text{CHCO} + \text{OH} \rightarrow .72 \text{CO} + .72 \text{CH}_3\text{CHO} + .72 \text{HO}_2 + .21 \text{CH}_3\text{COCO}_2\text{H} + .07 \text{CH}_3\text{CHO} + .07 \text{HO}_2 + .07 \text{CO}_2$ | $7.6\text{E-}11$ | Hatakeyama et al. (1985), Taraborrelli (2016) |
| G43047 | TrGCN | $\text{PROPOLNO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$ | $k_{t*f_{ono2*f_{pch2oh}+k_{s*f_{soh*f_{ch2ono2}}})}$ | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|--|
| G43048 | TrGCN | $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$ | $2.3\text{E}-12*\text{EXP}(300./\text{temp})$ | Tyndall et al. (2001a)* |
| G43049 | TrGCN | $\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2$ | $1.9\text{E}16*\text{EXP}(-10830./\text{temp})$ | Sehested et al. (1998)* |
| G43050 | TrGCN | $\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$ | $9.50\text{E}-13*\text{EXP}(-650./\text{temp})*\text{f_co}$ | Taraborrelli (2016)* |
| G43051a | TrGC | $\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$ | $0.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G43051b | TrGC | $\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$ | $k_{\text{s*f_sooh}}$ | Taraborrelli (2016) |
| G43051c | TrGC | $\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$ | $k_{\text{s*f_pch2oh}}$ | Taraborrelli (2016)* |
| G43052 | TrGC | $\text{C}_2\text{H}_5\text{CHO} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$ | $4.9\text{E}-12*\text{EXP}(405./\text{temp})$ | Atkinson et al. (2006)* |
| G43053 | TrGCN | $\text{C}_2\text{H}_5\text{CHO} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HNO}_3$ | $6.3\text{E}-15$ | Atkinson et al. (2006) |
| G43054a | TrGC | $\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$ | $k1_{\text{R02RC03}*0.9}$ | Taraborrelli (2016) |
| G43054b | TrGC | $\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$ | $k1_{\text{R02RC03}*0.1}$ | Taraborrelli (2016) |
| G43055a | TrGC | $\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{KAPH02}*rco3_oh$ | Taraborrelli (2016), Groß et al. (2014) |
| G43055b | TrGC | $\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$ | $\text{KAPH02}*rco3_ooh$ | Taraborrelli (2016), Groß et al. (2014) |
| G43055c | TrGC | $\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$ | $\text{KAPH02}*rco3_o3$ | Taraborrelli (2016), Groß et al. (2014) |
| G43056 | TrGCN | $\text{C}_2\text{H}_5\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43057 | TrGCN | $\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$ | $k_{\text{CH3CO3_NO2}}$ | Rickard and Pascoe (2009) |
| G43058 | TrGCN | $\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$ | $k_{\text{PAN_M}}$ | Rickard and Pascoe (2009) |
| G43059 | TrGC | $\text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$ | $k_{\text{co2h}}+k_{\text{p}}+k_{\text{s*f_co2h}}$ | Taraborrelli (2016)* |
| G43060a | TrGC | $\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$ | $0.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G43060b | TrGC | $\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$ | $k_{\text{s*f_co2h}}+k_{\text{p}}$ | Taraborrelli (2016)* |
| G43061 | TrGCN | $\text{PPN} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{s*f_cpan}}+k_{\text{p}}$ | Taraborrelli (2016)* |
| G43062 | TrGC | $\text{CH}_3\text{COCO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_3 + \text{H}_2\text{O}$ | $0.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G43063a | TrGC | $\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{OH}$ | $\text{KAPH02}*rco3_oh$ | Taraborrelli (2016) |
| G43063b | TrGC | $\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$ | $\text{KAPH02}*(rco3_ooh+rco3_o3)$ | Taraborrelli (2016) |
| G43064 | TrGCN | $\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_2$ | KAPNO | Taraborrelli (2016) |
| G43065 | TrGCN | $\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_3$ | $k_{\text{CH3CO3_NO2}}$ | Taraborrelli (2016)* |
| G43066 | TrGCN | $\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2 + \text{NO}_2$ | $\text{KR02N03}*1.74$ | Taraborrelli (2016) |
| G43067 | TrGC | $\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2$ | $k1_{\text{R02RC03}}$ | Taraborrelli (2016) |
| G43068 | TrGC | $\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{CO} + \text{HO}_2$ | $2.*k_{\text{t*f_co*f_o}}$ | Taraborrelli (2016) |
| G43069 | TrGC | $\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$ | $2.6\text{E}-12*\text{EXP}(200./\text{temp})$ | Atkinson et al. (2006) |
| G43070a | TrGC | $\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$ | $4.6\text{E}-12*\text{EXP}(70./\text{temp})*(k_{\text{s*f_soh}}/(k_{\text{p}}+k_{\text{s*f_pch2oh}}+k_{\text{s*f_soh}}))$ | Atkinson et al. (2006), Taraborrelli (2016)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| G43070b | TrGC | $\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO2} + \text{H}_2\text{O}$ | $4.6\text{E-}12 * \text{EXP}(70./\text{temp}) * ((k_p + k_s * f_pch2oh) / (k_p + k_s * f_pch2oh + k_s * f_soh))$ | Atkinson et al. (2006), Taraborrelli (2016)* |
| G43071a | TrGC | $\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$ | $k_CH2CHOH_OH_HCOOH$ | Taraborrelli (2016), So et al. (2014)* |
| G43072 | TrGC | $\text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCOOH}$ | $k_CH2CHOH_HCOOH$ | Taraborrelli (2016), daSilva (2010)* |
| G43073 | TrGC | $\text{C}_2\text{H}_5\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH}$ | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G43074 | TrGC | $\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$ | $k_s * f_sooh * f_co + .6 * k_CH3OOH_OH$ | Taraborrelli (2016)* |
| G43202 | TrGTerC | $\text{HCOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{CO}_3$ | 4.29E-11 | Rickard and Pascoe (2009) |
| G43203 | TrGTerCN | $\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$ | $2 * \text{KN03AL} * 2.4$ | Rickard and Pascoe (2009) |
| G43204a | TrGTerC | $\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$ | $k1_R02RC03 * 0.9$ | Taraborrelli (2016) |
| G43204b | TrGTerC | $\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$ | $k1_R02RC03 * 0.1$ | Taraborrelli (2016) |
| G43205 | TrGTerCN | $\text{HCOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43206 | TrGTerCN | $\text{HCOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN2}$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43207a | TrGTerC | $\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$ | $\text{KAPH02} * rco3_ooh$ | Rickard and Pascoe (2009) |
| G43207b | TrGTerC | $\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$ | $\text{KAPH02} * rco3_o3$ | Rickard and Pascoe (2009) |
| G43207c | TrGTerC | $\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{KAPH02} * rco3_oh$ | Rickard and Pascoe (2009) |
| G43210 | TrGTerCN | $\text{C}_3\text{PAN2} \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43211 | TrGTerCN | $\text{C}_3\text{PAN2} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$ | 2.10E-11 | Rickard and Pascoe (2009) |
| G43212 | TrGTerC | $\text{HCOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$ | 2.14E-11 | Rickard and Pascoe (2009) |
| G43213a | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$ | $k1_R02RC03 * 0.9$ | Taraborrelli (2016) |
| G43213b | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$ | $k1_R02RC03 * 0.1$ | Taraborrelli (2016) |
| G43214 | TrGTerCN | $\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G43215a | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$ | $\text{KAPH02} * rco3_ooh$ | Rickard and Pascoe (2009) |
| G43215b | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{KAPH02} * rco3_oh$ | Rickard and Pascoe (2009) |
| G43215c | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{O}_3$ | $\text{KAPH02} * rco3_o3$ | Rickard and Pascoe (2009) |
| G43218 | TrGTerCN | $\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN1}$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43219 | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$ | 1.39E-11 | Rickard and Pascoe (2009) |
| G43220 | TrGTerC | $\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3$ | 1.73E-11 | Rickard and Pascoe (2009) |
| G43221 | TrGTerCN | $\text{C}_3\text{PAN1} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43222 | TrGTerCN | $\text{C}_3\text{PAN1} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{CO} + \text{NO}_2$ | 4.51E-12 | Rickard and Pascoe (2009) |
| G43223 | TrGTerC | $\text{HCOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$ | 2.49E-11 | Rickard and Pascoe (2009)* |
| G43415 | TrGAroC | $\text{C3DIALOOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{OH}$ | 1.44E-10 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|---|---|
| G43418a | TrGAroC | $C3DIALO2 + HO_2 \rightarrow C3DIALOOH$ | $KR02H02(3)*(rco3_ooh+rco3_o3)$ | Rickard and Pascoe (2009) |
| G43418b | TrGAroC | $C3DIALO2 + HO_2 \rightarrow GLYOX + CO + HO_2 + OH$ | $KR02H02(3)*rco3_oh$ | Rickard and Pascoe (2009) |
| G43419 | TrGAroCN | $C3DIALO2 + NO \rightarrow GLYOX + CO + HO_2 + NO_2$ | $KR02NO$ | Rickard and Pascoe (2009)* |
| G43420 | TrGAroCN | $C3DIALO2 + NO_3 \rightarrow GLYOX + CO + HO_2 + NO_2$ | $KR02NO3$ | Rickard and Pascoe (2009)* |
| G43421 | TrGAroC | $C3DIALO2 \rightarrow GLYOX + CO + HO_2$ | $k1_R02s0R02$ | Rickard and Pascoe (2009)* |
| G43422a | TrGAroC | $HCOCOHCO3 + HO_2 \rightarrow GLYOX + CO_2 + HO_2 + OH$ | $KAPH02*rco3_oh$ | Rickard and Pascoe (2009) |
| G43422b | TrGAroC | $HCOCOHCO3 + HO_2 \rightarrow HCOCOHCO3H$ | $KAPH02*(rco3_ooh+rco3_o3)$ | Rickard and Pascoe (2009) |
| G43424 | TrGAroCN | $HCOCOHCO3 + NO \rightarrow GLYOX + CO_2 + HO_2 + NO_2$ | $KAPNO$ | Rickard and Pascoe (2009) |
| G43425 | TrGAroCN | $HCOCOHCO3 + NO_2 \rightarrow HCOCOH PAN$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G43426 | TrGAroCN | $HCOCOHCO3 + NO_3 \rightarrow GLYOX + CO_2 + HO_2 + NO_2$ | $KR02NO3*1.74$ | Rickard and Pascoe (2009) |
| G43427 | TrGAroC | $HCOCOHCO3 \rightarrow GLYOX + CO_2 + HO_2$ | $k1_R02RCO3$ | Rickard and Pascoe (2009) |
| G43428 | TrGAroC | $METACETHO + OH \rightarrow CH_3C(O) + CO_2$ | $9.82E-11$ | Rickard and Pascoe (2009) |
| G43442 | TrGAroCN | $HCOCOH PAN + OH \rightarrow GLYOX + CO + NO_2$ | $6.97E-11$ | Rickard and Pascoe (2009) |
| G43443 | TrGAroCN | $HCOCOH PAN \rightarrow HCOCOHCO3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G43444 | TrGAroC | $C32OH13CO + OH \rightarrow HCOCOHCO3$ | $1.36E-10$ | Rickard and Pascoe (2009) |
| G43446 | TrGAroC | $HCOCOHCO3H + OH \rightarrow HCOCOHCO3$ | $7.33E-11$ | Rickard and Pascoe (2009) |
| G44000 | TrGC | $C_4H_{10} + OH \rightarrow LC_4H_9O_2 + H_2O$ | $2.03E-17*temp*temp*EXP(78./temp)$ | Atkinson et al. (2006)* |
| G44001a | TrGC | $LC_4H_9O_2 \rightarrow C_3H_7CHO + HO_2$ | $(k1_R02pR02*0.1273+k1_R02sR02*0.8727)*0.1273$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44001b | TrGC | $LC_4H_9O_2 \rightarrow .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 C_2H_5O_2$ | $(k1_R02pR02*0.1273+k1_R02sR02*0.8727)*0.8727$ | Rickard and Pascoe (2009), Taraborrelli (2016)* |
| G44002 | TrGC | $LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$ | $KR02H02(4)$ | Rickard and Pascoe (2009) |
| G44003a | TrGCN | $LC_4H_9O_2 + NO \rightarrow NO_2 + C_3H_7CHO + HO_2$ | $KR02NO*(1-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.1273$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44003b | TrGCN | $LC_4H_9O_2 + NO \rightarrow NO_2 + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 C_2H_5O_2$ | $KR02NO*(1-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.8727$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44003c | TrGCN | $LC_4H_9O_2 + NO \rightarrow LC_4H_9NO_3$ | $KR02NO*(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair))$ | Rickard and Pascoe (2009)* |
| G44004a | TrGCN | $LC_4H_9O_2 + NO_3 \rightarrow NO_2 + C_3H_7CHO + HO_2$ | $KR02NO3*0.1273$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44004b | TrGCN | $LC_4H_9O_2 + NO_3 \rightarrow NO_2 + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 C_2H_5O_2$ | $KR02NO3*0.8727$ | Rickard and Pascoe (2009), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|---|
| G44005a | TrGC | $\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G44005b | TrGC | $\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$ | $k_{\text{s}} \cdot f_{\text{tooh}} \cdot f_{\text{alk}} \cdot (k_{\text{p}} / (k_{\text{p}} + k_{\text{s}}))$ | Taraborrelli (2016) |
| G44005c | TrGC | $\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$ | $k_{\text{t}} \cdot f_{\text{tooh}} \cdot f_{\text{alk}} \cdot (k_{\text{s}} / (k_{\text{p}} + k_{\text{s}}))$ | Taraborrelli (2016) |
| G44006a | TrGC | $\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | $1.17\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp})$ | Atkinson (2003) |
| G44006b | TrGC | $\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | $*k_{\text{t}} / (3 \cdot k_{\text{p}} + k_{\text{t}})$ $1.17\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp})$ | Atkinson (2003) |
| G44007 | TrGC | $\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$ | $*3 \cdot k_{\text{p}} / (3 \cdot k_{\text{p}} + k_{\text{t}})$ $k1_{\text{R02tR02}}$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44008 | TrGC | $\text{TC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{TC}_4\text{H}_9\text{OOH}$ | $\text{KR02H02}(4)$ | Rickard and Pascoe (2009) |
| G44009a | TrGCN | $\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$ | $\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 3, 0, 0, 0, \text{temp}, \text{cair}))$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44009b | TrGCN | $\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC4H9NO3}$ | $\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 3, 0, 0, 0, \text{temp}, \text{cair})$ | Rickard and Pascoe (2009) |
| G44010a | TrGC | $\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G44010b | TrGC | $\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$ | $3 \cdot k_{\text{p}} \cdot f_{\text{tch2oh}}$ | Taraborrelli (2016)* |
| G44011 | TrGCN | $\text{TC4H9NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$ | $3 \cdot k_{\text{p}} \cdot f_{\text{ch2ono2}}$ | Taraborrelli (2016)* |
| G44012 | TrGC | $\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$ | $k1_{\text{R02sR02}}$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44013 | TrGC | $\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$ | $\text{KR02H02}(4)$ | Rickard and Pascoe (2009) |
| G44014a | TrGCN | $\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$ | $\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44014b | TrGCN | $\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC4H9NO3}$ | $\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair})$ | Rickard and Pascoe (2009) |
| G44015a | TrGC | $\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G44015b | TrGC | $\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$ | $k_{\text{s}} \cdot f_{\text{sooh}} + 2 \cdot k_{\text{s}} + k_{\text{t}} \cdot f_{\text{pch2oh}}$ | Taraborrelli (2016)* |
| G44016 | TrGCN | $\text{IC4H9NO3} + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{s}} \cdot f_{\text{ono2}} + 2 \cdot k_{\text{p}} + k_{\text{t}} \cdot f_{\text{ch2ono2}}$ | Taraborrelli (2016)* |
| G44017 | TrGC | $\text{MVK} + \text{O}_3 \rightarrow .87 \text{ MGLYOX} + .5481 \text{ CO} + .1392 \text{ HO}_2$ $+ .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .13 \text{ HCHO} + .04680 \text{ OH}$ $+ .04680 \text{ CO} + .07280 \text{ CH}_3\text{C(O)} + .026 \text{ CH}_3\text{CHO} + .026$ $\text{CO}_2 + .026 \text{ HCHO} + .026 \text{ HO}_2 + .02402 \text{ MGLYOX} +$ $.02402 \text{ H}_2\text{O}_2 + .00718 \text{ CH}_3\text{COCO}_2\text{H}$ | $8.5\text{E-}16 \cdot \text{EXP}(-1520./\text{temp})$ | Taraborrelli (2016) |
| G44018 | TrGC | $\text{MVK} + \text{OH} \rightarrow \text{LHMVKABO2}$ | $2.6\text{E-}12 \cdot \text{EXP}(610./\text{temp})$ | Taraborrelli (2016), Atkinson et al. (2006)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|--|
| G44019 | TrGC | MEK + OH → LMEKO2 + H ₂ O | 1.5E-12*EXP(-90./temp) | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44020 | TrGC | LMEKO2 + HO ₂ → LMEKOOH | KR02H02(4) | Taraborrelli (2016) |
| G44021a | TrGCN | LMEKO2 + NO → .62 CH ₃ CHO + .62 CH ₃ C(O) + .38 HCHO + .38 CO ₂ + .38 HOCH ₂ CH ₂ O ₂ + NO ₂ | KR02N0*(1-(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair))) | Taraborrelli (2016)* |
| G44021b | TrGCN | LMEKO2 + NO → LMEKNO3 | KR02N0*(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair)) | Taraborrelli (2016) |
| G44022a | TrGC | LMEKOOH + OH → LMEKO2 + H ₂ O | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G44022b | TrGC | LMEKOOH + OH → .62 BIACET + .38 HCHO + .38 CO ₂ + .38 HOCH ₂ CH ₂ O ₂ + H ₂ O + OH | (.62*k_t*f_tooh*f_co+.38*k_s*f_sooH) | Taraborrelli (2016) |
| G44023a | TrGCN | LC4H9NO3 + OH → MEK + NO ₂ + H ₂ O | (k_t*f_ono2*f_alk+k_p*f_alk+k_s*f_ch2ono2+k_p)*(k_s/(k_p+k_s)) | Taraborrelli (2016)* |
| G44023b | TrGCN | LC4H9NO3 + OH → C ₃ H ₇ CHO + NO ₂ + H ₂ O | (k_p+k_s*(1+f_ch2ono2+f_ono2)*f_alk)*(k_p/(k_p+k_s)) | Taraborrelli (2016)* |
| G44024 | TrGCN | MPAN + OH → CH ₃ COCH ₂ OH + 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 ₂ CH ₂ O ₂ + .079 C ₂ H ₅ O ₂ + .462 CH ₃ C(O) + .462 CH ₃ CHO | (.62*k1_R02s0R02+.38*k1_R02p0R02) | Rickard and Pascoe (2009)* |
| G44027 | TrGC | MACR + OH → .45 MACO3 + .55 MACRO2 | 8.E-12*EXP(380./temp) | Orlando et al. (1999b), Taraborrelli (2016) |
| G44028 | TrGC | MACR + O ₃ → .5481 CO + .1392 HO ₂ + .1392 OH + .3219 CH ₂ OO + .87 MGLYOX + .13 HCHO + .13 OH + .065 HCOCOCH ₂ O ₂ + .065 CO + .065 CH ₃ C(O) | 1.36E-15*EXP(-2112./temp) | Taraborrelli (2016) |
| G44029 | TrGCN | MACR + NO ₃ → MACO3 + HNO ₃ | KN03AL*2.0 | Rickard and Pascoe (2009) |
| G44030a | TrGC | MACO3 → CH ₃ C(O) + HCHO + CO ₂ | k1_R02RC03*0.9 | Taraborrelli (2016) |
| G44030b | TrGC | MACO3 → MACO2H | k1_R02RC03*0.1 | Taraborrelli (2016) |
| G44031a | TrGC | MACO3 + HO ₂ → MACO2 + OH | KAPH02*rco3_oh | Taraborrelli (2016) |
| G44031b | TrGC | MACO3 + HO ₂ → MACO3H | KAPH02*rco3_ooh | Taraborrelli (2016) |
| G44031c | TrGC | MACO3 + HO ₂ → MACO2H + O ₃ | KAPH02*rco3_o3 | Taraborrelli (2016) |
| G44032 | TrGCN | MACO3 + NO → MACO2 + NO ₂ | 8.70E-12*EXP(290./temp) | Taraborrelli (2016) |
| G44033 | TrGCN | MACO3 + NO ₂ → MPAN | k_CH3C03_NO2 | Rickard and Pascoe (2009) |
| G44034 | TrGCN | MACO3 + NO ₃ → MACO2 + NO ₂ | KR02N03*1.60 | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|----------------------------|
| G44035 | TrGC | MACRO2 \rightarrow .7 CH ₃ COCH ₂ OH + .7 HCHO + .7 HO ₂ + .3 MACROH | k1_R02t0R02 | Rickard and Pascoe (2009)* |
| G44036a | TrGC | MACRO2 + HO ₂ \rightarrow MACRO + OH | KR02H02(4)*rcoch2o2_oh | Taraborrelli (2016) |
| G44036b | TrGC | MACRO2 + HO ₂ \rightarrow MACROOH | KR02H02(4)*rcoch2o2_ooH | Taraborrelli (2016) |
| G44037a | TrGCN | MACRO2 + NO \rightarrow MACRO + NO ₂ | KR02N0*(1.-alpha_AN(6,3,1,0,0,temp,cair)) | Taraborrelli (2016) |
| G44037b | TrGCN | MACRO2 + NO \rightarrow MACRN | KR02N0*alpha_AN(6,3,1,0,0,temp,cair) | Taraborrelli (2016) |
| G44038 | TrGCN | MACRO2 + NO ₃ \rightarrow MACRO + NO ₂ | KR02N03 | Taraborrelli (2016) |
| G44039a | TrGC | MACROOH + OH \rightarrow MACRO2 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G44039b | TrGC | MACROOH + OH \rightarrow CO + CH ₃ COCH ₂ OH + OH | k_t*f_o*f_tch2oh*f_alk | Taraborrelli (2016) |
| G44039c | TrGC | MACROOH + OH \rightarrow CO + MGLYOX + HO ₂ | (k_s*f_soh*f_pch2oh + k_rohro) | Taraborrelli (2016) |
| G44040 | TrGC | MACROH + OH \rightarrow CH ₃ COCH ₂ OH + CO + HO ₂ | k_t*f_o*f_tch2oh*f_alk | Taraborrelli (2016) |
| G44041 | TrGC | MACRO \rightarrow .885 CH ₃ COCH ₂ OH + .885 CO + .115 MGLYOX + .115 HCHO + HO ₂ | KDEC | Taraborrelli (2016) |
| G44042 | TrGC | MACO2H + OH \rightarrow CH ₃ COCH ₂ OH + HO ₂ + CO ₂ | ((k_adt+k_adp)*a_co2h+k_co2h) | Taraborrelli (2016) |
| G44043a | TrGC | MACO3H + OH \rightarrow CH ₃ COCH ₂ OH + CO ₂ + OH | (k_adt+k_adp)*a_co2h | Taraborrelli (2016) |
| G44043b | TrGC | MACO3H + OH \rightarrow MACO3 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G44044 | TrGC | LHMKABO2 \rightarrow .024 CO2H3CHO + .072 MGLYOX + .072 HO ₂ + .072 HCHO + .5280 CH ₃ C(O) + .5280 HOCH ₂ CHO + .176 BIACETOH + .2 HO12CO3C4 | (.12*k1_R02p0R02+.88*k1_R02s0R02) | Taraborrelli (2016) |
| G44045a | TrGC | LHMKABO2 + HO ₂ \rightarrow OH + HOCH ₂ CHO + CH ₃ C(O) | KR02H02(4)*.88*rcoch2o2_oh | Taraborrelli (2016) |
| G44045b | TrGC | LHMKABO2 + HO ₂ \rightarrow LHMKABOOH | KR02H02(4)*(.12+.88*rcoch2o2_ooH) | Taraborrelli (2016) |
| G44046a | TrGCN | LHMKABO2 + NO \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + NO ₂ | KR02N0*(1.-(.12*alpha_AN(6,1,0,1,0,temp,cair))+.88*alpha_AN(6,2,1,0,0,temp,cair))) | Taraborrelli (2016) |
| G44046b | TrGCN | LHMKABO2 + NO \rightarrow MVKNO3 | KR02N0*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)) | Taraborrelli (2016)* |
| G44047 | TrGCN | LHMKABO2 + NO ₃ \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + .12 HO ₂ + NO ₂ | KR02N03 | Taraborrelli (2016) |
| G44048a | TrGC | LHMKABOOH + OH \rightarrow LHMKABO2 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G44048b | TrGC | LHMKABOOH + OH \rightarrow .12 CO2H3CHO + .88 BIACETOH + OH | (.12*k_s*f_soh*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co) | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|---|---------------------------|
| G44049a | TrGC | $\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$ | $k_{\text{t*f}_o\text{*f}_\text{alk}}$ | Taraborrelli (2016) |
| G44049b | TrGC | $\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{H}_2\text{O}$ | $k_{\text{t*f}_\text{co*f}_\text{toh*f}_\text{cho}}$ | Taraborrelli (2016) |
| G44050 | TrGCN | $\text{CO}_2\text{H}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{HNO}_3$ | KN03AL*4.0 | Rickard and Pascoe (2009) |
| G44051 | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$ | $k_{1_R02RC03}$ | Taraborrelli (2016) |
| G44052a | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$ | KAPH02*rco3_oh | Taraborrelli (2016) |
| G44052b | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{O}_3$ | KAPH02*rco3_o3 | Taraborrelli (2016) |
| G44052c | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3\text{H}$ | KAPH02*rco3_ooh | Taraborrelli (2016) |
| G44053 | TrGCN | $\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$ | KAPNO | Taraborrelli (2016) |
| G44054 | TrGCN | $\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$ | KR02N03*1.60 | Taraborrelli (2016) |
| G44055a | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$ | $0.6*k_{\text{CH300H_OH}}$ | Taraborrelli (2016) |
| G44055b | TrGC | $\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{CO}_2 + \text{OH}$ | $(k_{\text{t*f}_\text{co2h*f}_\text{co*f}_\text{toh}})$ | Taraborrelli (2016) |
| G44056 | TrGC | $\text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCOCO}_2\text{H} + \text{HO}_2$ | $k_{\text{t*f}_\text{co2h*f}_\text{co*f}_\text{toh}+k_{\text{co2h}}}$ | Taraborrelli (2016) |
| G44057a | TrGC | $\text{HO}_12\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{BIACETOH} + \text{HO}_2$ | $k_{\text{t*f}_\text{toh*f}_\text{alk*f}_\text{co}}$ | Taraborrelli (2016) |
| G44057b | TrGC | $\text{HO}_12\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$ | $k_{\text{s*f}_\text{soh*f}_\text{alk}}$ | Taraborrelli (2016) |
| G44058 | TrGC | $\text{MACO}_2 \rightarrow .65 \text{CH}_3 + .65 \text{CO} + .65 \text{HCHO} + .35 \text{OH} + .35 \text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$ | KDEC | Taraborrelli (2016) |
| G44059 | TrGC | $\text{LHMVKABO}_2 \rightarrow .88 \text{MGLYOX} + .88 \text{HCHO} + .12 \text{HOOCH}_2\text{CHO} + .12 \text{CH}_3\text{C(O)} + \text{OH}$ | KHSD | Taraborrelli (2016) |
| G44060 | TrGC | $\text{MACRO}_2 \rightarrow \text{MGLYOX} + \text{HCHO} + \text{OH}$ | KHSB | Taraborrelli (2016) |
| G44061a | TrGCN | $\text{MVKNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{s*f}_\text{sooh*f}_\text{ch2ono2}+k_{\text{rohro}}}$ | Taraborrelli (2016)* |
| G44061b | TrGCN | $\text{MVKNO}_3 + \text{OH} \rightarrow \text{BIACETOH} + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{t*f}_\text{ono2*f}_\text{co*f}_\text{pch2oh}}$ | Taraborrelli (2016)* |
| G44062a | TrGCN | $\text{MACRN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{t*f}_\text{o*f}_\text{ch2ono2}}$ | Taraborrelli (2016)* |
| G44062b | TrGCN | $\text{MACRN} + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$ | $k_{\text{rohro}+k_{\text{s*f}_\text{sooh*f}_\text{ch2ono2}}}$ | Taraborrelli (2016)* |
| G44063 | TrGC | $\text{MACRO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH} + \text{CO}$ | K14HSAL | Taraborrelli (2016) |
| G44064 | TrGC | $\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow .9 \text{CH}_3\text{COCHCO} + .1 \text{CH}_3\text{C(O)} + .01 \text{GLYOX} + .18 \text{CO} + .09 \text{HO}_2 + \text{OH}$ | K15HS24VYNAL | Taraborrelli (2016) |
| G44065 | TrGC | $\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOHCHCHO}$ | KR02H02(4) | Taraborrelli (2016) |
| G44066 | TrGCN | $\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$ | KR02NO | Taraborrelli (2016)* |
| G44067 | TrGCN | $\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$ | kr02N03 | Taraborrelli (2016) |
| G44068 | TrGC | $\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO}$ | $k_{1_R02s0R02}$ | Taraborrelli (2016) |
| G44069 | TrGC | $\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCCH}_3\text{CO} + \text{OH}$ | K15HS24VYNAL | Taraborrelli (2016) |
| G44070 | TrGCN | $\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$ | KR02NO | Taraborrelli (2016)* |
| G44071 | TrGC | $\text{EZCHOCCH}_3\text{CHO}_2 + \text{HO}_2 \rightarrow \text{HCOCCH}_3\text{CHOOH}$ | KR02H02(4) | Taraborrelli (2016) |
| G44072 | TrGCN | $\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO}_3 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|--|
| G44073 | TrGC | $\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO}$ | k1_R02p0R02 | Taraborrelli (2016) |
| G44074 | TrGC | $\text{CH}_3\text{COOHCHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{OH}$ | KHYDEC | Taraborrelli (2016) |
| G44075 | TrGC | $\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{OH}$ | KHYDEC | Taraborrelli (2016) |
| G44076 | TrGCN | $\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G44077 | TrGCN | $\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G44078 | TrGC | $\text{CH}_3\text{COCHO}_2\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{OH}$ | KR02H02(4) | Taraborrelli (2016)* |
| G44079 | TrGC | $\text{CH}_3\text{COCHO}_2\text{CHO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX}$ | k1_R02s0R02 | Taraborrelli (2016) |
| G44080 | TrGC | $\text{HCOCO}_2\text{CH}_3\text{CHO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$ | k1_R02t0R02 | Taraborrelli (2016) |
| G44081 | TrGCN | $\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G44082 | TrGC | $\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$ | KR02H02(4) | Taraborrelli (2016)* |
| G44083 | TrGCN | $\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G44084 | TrGC | $\text{HCOCCH}_3\text{CO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$ | 1E-10*a_cho | Hatakeyama et al. (1985), Taraborrelli (2016) |
| G44085 | TrGC | $\text{CH}_3\text{COCHCO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$ | 7.6E-11*a_coch3 | Hatakeyama et al. (1985), Taraborrelli (2016)* |
| G44086 | TrGCN | $\text{LMEKNO}_3 + \text{OH} \rightarrow .62 \text{MGLYOX} + .62 \text{HCHO} + .62 \text{HO}_2 + .62 \text{NO}_2 + .38 \text{CH}_3\text{C}(\text{O}) + .38 \text{NO}_3\text{CH}_2\text{CHO}$ | .62*(k_p*(f_co+f_ch2ono2)) +.38*(k_s*f_ch2ono2*f_co) | Taraborrelli (2016)* |
| G44087 | TrGC | $\text{MEPROPENE} + \text{OH} \rightarrow \text{IBUTOLBO}_2$ | 9.4E-12*EXP(505./temp) | Atkinson et al. (2006) |
| G44088a | TrGC | $\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_2\text{OO}^*$ | 2.7E-15*EXP(-1630./temp)*0.33 | Atkinson et al. (2006), Taraborrelli (2016) |
| G44088b | TrGC | $\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{OH} + \text{HCHO}$ | 2.7E-15*EXP(-1630./temp)*0.67 | Atkinson et al. (2006), Taraborrelli (2016) |
| G44089 | TrGCN | $\text{MEPROPENE} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2$ | 3.4E-13 | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44090 | TrGC | $\text{IBUTOLBO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$ | k1_R02t0R02 | Taraborrelli (2016) |
| G44091a | TrGC | $\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{IBUTOLBOOH}$ | KR02H02(4)*rcoch2o2_ooH | Taraborrelli (2016) |
| G44091b | TrGC | $\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$ | KR02H02(4)*rcoch2o2_oh | Taraborrelli (2016) |
| G44092a | TrGCN | $\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | KR02N0*(1.-alpha_AN(5,3,0,0,0, temp, cair)) | Taraborrelli (2016) |
| G44092b | TrGCN | $\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{IBUTOLBNO}_3$ | KR02N0*alpha_AN(5,3,0,0,0, temp, cair) | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|--|
| G44093 | TrGCN | $\text{IBUTOLBO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G44094a | TrGC | $\text{IBUTOLBOOH} + \text{OH} \rightarrow \text{IBUTOLBO2}$ | .6*k_CH300H_OH | Taraborrelli (2016) |
| G44094b | TrGC | $\text{IBUTOLBOOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$ | k_s*f_sooh*f_pch2oh | Taraborrelli (2016) |
| G44095 | TrGCN | $\text{IBUTOLBNO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | 3.*k_p | Taraborrelli (2016) |
| G44096 | TrGC | $\text{BUT1ENE} + \text{OH} \rightarrow \text{LBUT1ENO2}$ | 6.6E-12*EXP(465./temp) | Atkinson et al. (2006)* |
| G44097a | TrGC | $\text{BUT1ENE} + \text{O}_3 \rightarrow \text{HCHO} + .5 \text{C}_2\text{H}_5\text{CHO} + .5 \text{H}_2\text{O}_2 + .5 \text{CH}_3\text{CHO} + .5 \text{CO} + .5 \text{HO}_2$ | 3.35E-15*EXP(-1745./temp)*.57 | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44097b | TrGC | $\text{BUT1ENE} + \text{O}_3 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{CH}_2\text{OO}^*$ | 3.35E-15*EXP(-1745./temp)*.43 | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44098 | TrGCN | $\text{BUT1ENE} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{NO}_2$ | 3.2E-13*EXP(-950./temp) | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44099 | TrGC | $\text{LBUT1ENO2} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2$ | k1_R02s0R02 | Taraborrelli (2016) |
| G44100a | TrGC | $\text{LBUT1ENO2} + \text{HO}_2 \rightarrow \text{LBUT1ENOOH}$ | KR02H02(4)*rcoch2o2_ooh | Taraborrelli (2016) |
| G44100b | TrGC | $\text{LBUT1ENO2} + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$ | KR02H02(4)*rcoch2o2_oh | Taraborrelli (2016) |
| G44101a | TrGCN | $\text{LBUT1ENO2} + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | KR02N0*(1.-alpha_AN(5,2,0,0,0,temp,cair)) | Taraborrelli (2016) |
| G44101b | TrGCN | $\text{LBUT1ENO2} + \text{NO} \rightarrow \text{LBUT1ENNO3}$ | KR02N0*alpha_AN(5,2,0,0,0,temp,cair) | Taraborrelli (2016) |
| G44102 | TrGCN | $\text{LBUT1ENO2} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G44103a | TrGC | $\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{LBUT1ENO2}$ | .6*k_CH300H_OH | Taraborrelli (2016) |
| G44103b | TrGC | $\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HCHO} + \text{HO}_2$ | k_t*f_tooh*f_pch2oh | Taraborrelli (2016)* |
| G44104 | TrGCN | $\text{LBUT1ENNO3} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$ | k_s*f_soh*f_ch2ono2 | Taraborrelli (2016)* |
| G44105 | TrGC | $\text{CBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$ | 1.1E-11*EXP(485./temp) | Atkinson et al. (2006) |
| G44106 | TrGC | $\text{CBUT2ENE} + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + .16 \text{CH}_3\text{CHOHOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$ | 3.2E-15*EXP(-965./temp) | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44107 | TrGCN | $\text{CBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{CH}_3\text{CHO} + \text{NO}_2$ | 3.5E-13 | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44108 | TrGC | $\text{TBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$ | 1.0E-11*EXP(553./temp) | Atkinson et al. (2006) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|--|
| G44109 | TrGC | TBUT2ENE + O ₃ → CH ₃ CHO + .16 CH ₃ CHOHOOH + .50 OH + .50 HCOCH ₂ O ₂ + .05 CH ₂ CO + .09 CH ₃ OH + .09 CO + .2 CH ₄ + .2 CO ₂ | 6.6E-15*EXP(-1060./temp) | Atkinson et al. (2006), Taraborrelli (2016) |
| G44110 | TrGCN | TBUT2ENE + NO ₃ → 2 CH ₃ CHO + NO ₂ | 1.78E-12*EXP(-530./temp) +1.28E-14*EXP(570./temp) | Atkinson et al. (2006), Taraborrelli (2016)* |
| G44111 | TrGC | BUT2OLO2 → C ₂ H ₅ CHO + HCHO + HO ₂ | k1_R02s0R02 | Taraborrelli (2016) |
| G44112a | TrGC | BUT2OLO2 + HO ₂ → BUT2OLOOH | KR02H02(4)*rcoch2o2_ooh | Taraborrelli (2016) |
| G44112b | TrGC | BUT2OLO2 + HO ₂ → 2 CH ₃ CHO + HO ₂ + OH | KR02H02(4)*rcoch2o2_oh | Taraborrelli (2016) |
| G44113a | TrGCN | BUT2OLO2 + NO → 2 CH ₃ CHO + HO ₂ + NO ₂ | KR02N0*(1.-alpha_AN(5,2,0,0,0, temp, cair)) | Taraborrelli (2016) |
| G44113b | TrGCN | BUT2OLO2 + NO → BUT2OLNO3 | KR02N0*alpha_AN(5,2,0,0,0,temp, cair) | Taraborrelli (2016) |
| G44114 | TrGCN | BUT2OLO2 + NO ₃ → 2 CH ₃ CHO + HO ₂ + NO ₂ | KR02N03 | Taraborrelli (2016) |
| G44115a | TrGC | BUT2OLOOH + OH → BUT2OLO2 | .6*k_CH300H_OH | Taraborrelli (2016) |
| G44115b | TrGC | BUT2OLOOH + OH → LMEKOOH + HO ₂ | k_t*f_toh*f_pch2oh | Taraborrelli (2016) |
| G44115c | TrGC | BUT2OLOOH + OH → BUT2OLO + OH | k_t*f_tooh*f_pch2oh | Taraborrelli (2016) |
| G44116 | TrGCN | BUT2OLNO3 + OH → LMEKNO3 + HO ₂ | k_t*f_toh*f_ch2ono2 | Taraborrelli (2016) |
| G44117 | TrGC | BUT2OLO + OH → BIACET + HO ₂ | k_t*f_toh*f_co | Taraborrelli (2016) |
| G44118 | TrGC | IPRCHO + OH → IPRCO3 + H ₂ O | 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 ₃ H ₇ O ₂ + CO ₂ | k1_R02RC03 | Rickard and Pascoe (2009) |
| G44121a | TrGC | IPRCO3 + HO ₂ → PERIBUACID | KAPH02*rco3_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44121b | TrGC | IPRCO3 + HO ₂ → iC ₃ H ₇ O ₂ + CO ₂ + OH | KAPH02*(1-rco3_ooh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44122 | TrGCN | IPRCO3 + NO ₂ → PIPN | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G44123 | TrGCN | IPRCO3 + NO → iC ₃ H ₇ O ₂ + CO ₂ + NO ₂ | KAPNO | Rickard and Pascoe (2009) |
| G44124a | TrGC | PERIBUACID + OH → IPRCO3 + H ₂ O | .6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G44124b | TrGC | PERIBUACID + OH → CH ₃ COCH ₃ + H ₂ O + CO ₂ | k_s*f_co2h | Taraborrelli (2016)* |
| G44125 | TrGCN | PIPn → IPRCO3 + NO ₂ | k_PAN_M | Rickard and Pascoe (2009) |
| G44126 | TrGCN | PIPn + OH → CH ₃ COCH ₃ + CO ₂ + NO ₂ | k_s*f_cpan | Taraborrelli (2016)* |
| G44127 | TrGC | MPROPENOL + OH → HCOOH + OH + CH ₃ COCH ₃ | k_CH2CHOH_OH_HCOOH | Taraborrelli (2016), So et al. (2014)* |
| G44128 | TrGC | MPROPENOL + HCOOH → IPRCHO + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|----------------------------------|---|
| G44129 | TrGC | IPRCHO + HCOOH → MPROPENOL + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44130 | TrGC | BUTENOL + OH → HCOOH + OH + C ₂ H ₅ CHO | k_CH2CHOH_OH_HCOOH | Taraborrelli (2016), So et al. (2014)* |
| G44131 | TrGC | BUTENOL + HCOOH → C ₃ H ₇ CHO + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44132 | TrGC | C ₃ H ₇ CHO + HCOOH → BUTENOL + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44133 | TrGC | HVMK + OH → HCOOH + OH + MGLYOX | 8.8E-11 | Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)* |
| G44134 | TrGC | HVMK + HCOOH → CO ₂ C ₃ CHO + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44135 | TrGC | CO ₂ C ₃ CHO + HCOOH → HVMK + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44136 | TrGC | HMAC + OH → HCOOH + OH + MGLYOX | 8.8E-11 | Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)* |
| G44137 | TrGC | HMAC + HCOOH → IBUTDIAL + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44138 | TrGC | IBUTDIAL + HCOOH → HMAC + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G44139 | TrGC | CO ₂ C ₃ CHO + OH → CH ₃ COCH ₂ O ₂ + CO ₂ + H ₂ O | k_t*f_o*f_alk+k_s*f_cho*f_co | Taraborrelli (2016)* |
| G44140 | TrGCN | CO ₂ C ₃ CHO + NO ₃ → CH ₃ COCH ₂ O ₂ + CO ₂ + HNO ₃ | KN03AL*4.0 | Taraborrelli (2016)* |
| G44141 | TrGC | IBUTDIAL + OH → CH ₃ CHO + CO + HO ₂ + CO ₂ + H ₂ O | 2.*k_t*f_o*f_alk+k_t*f_cho*f_cho | Taraborrelli (2016)* |
| G44142 | TrGCN | IBUTDIAL + NO ₃ → CH ₃ CHO + CO + HO ₂ + CO ₂ + HNO ₃ | 2.*KN03AL*4.0 | Taraborrelli (2016)* |
| G44200 | TrGTerC | CH ₃ COCOCH ₂ O ₂ → CH ₃ C(O) + HCHO + CO | k1_R02p0R02 | Rickard and Pascoe (2009) |
| G44201 | TrGTerC | CH ₃ COCOCH ₂ O ₂ + HO ₂ → CH ₃ COCOCH ₂ OOH | KR02HO2(4) | Rickard and Pascoe (2009) |
| G44202 | TrGTerCN | CH ₃ COCOCH ₂ O ₂ + NO → CH ₃ C(O) + HCHO + CO + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |
| G44203a | TrGTerC | CH ₃ COCOCH ₂ OOH + OH → CH ₃ COCOCHO + OH | k_s*f_co*f_sooh | Rickard and Pascoe (2009)* |
| G44203b | TrGTerC | CH ₃ COCOCH ₂ OOH + OH → CH ₃ COCOCH ₂ O ₂ | .6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G44204 | TrGTerC | C44O ₂ + HO ₂ → C44OOH | KR02HO2(4) | Rickard and Pascoe (2009) |
| G44205 | TrGTerCN | C44O ₂ + NO → HCOCH ₂ CHO + CO ₂ + HO ₂ + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |
| G44206 | TrGTerC | C44O ₂ → HCOCH ₂ CHO + CO ₂ + HO ₂ | k1_R02s0R02 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|---------------------------------|---|
| G44207 | TrGTerC | $C44OOH + OH \rightarrow C44O2$ | 7.46E-11 | Rickard and Pascoe (2009) |
| G44208 | TrGTerC | $CHOC3COO2 \rightarrow HCOCH2CO3 + HCHO$ | k1_R02p0R02 | Rickard and Pascoe (2009) |
| G44209 | TrGTerC | $CHOC3COO2 + HO_2 \rightarrow C413COOOH$ | KR02H02(4) | Rickard and Pascoe (2009) |
| G44210 | TrGTerCN | $CHOC3COO2 + NO \rightarrow HCOCH2CO3 + HCHO + NO_2$ | KR02N0 | 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.*KN03AL*4.0 | Rickard and Pascoe (2009) |
| G44214 | TrGTerC | $C312COCO3 \rightarrow HCOCOCH_2O_2 + CO_2$ | k1_R02RC03 | Rickard and Pascoe (2009) |
| G44215a | TrGTerC | $C312COCO3 + HO_2 \rightarrow C312COCO3H$ | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G44215b | TrGTerC | $C312COCO3 + HO_2 \rightarrow HCOCOCH_2O_2 + CO_2 + OH$ | KAPH02*(1-rco3_ooh) | Rickard and Pascoe (2009) |
| G44216 | TrGTerCN | $C312COCO3 + NO_2 \rightarrow C312COPAN$ | k_CH3C03_N02 | 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) | Taraborrelli (2016)* |
| G44222 | TrGTerCN | $CH_3COCOCHO + NO_3 \rightarrow CH_3C(O) + 2 CO + HNO_3$ | KN03AL*4.0 | Rickard and Pascoe (2009) |
| G44223 | TrGTerC | $IBUTALOH + OH \rightarrow IPRHOCO3$ | 1.4E-11 | Rickard and Pascoe (2009) |
| G44224a | TrGTerC | $IPRHOCO3 + HO_2 \rightarrow CH_3COCH_3 + CO_2 + HO_2 + OH$ | KAPH02*rco3_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44224b | TrGTerC | $IPRHOCO3 + HO_2 \rightarrow IPRHOCO2H + O_3$ | KAPH02*rco3_o3 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44224c | TrGTerC | $IPRHOCO3 + HO_2 \rightarrow IPRHOCO3H$ | KAPH02*rco3_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44225 | TrGTerCN | $IPRHOCO3 + NO \rightarrow CH_3COCH_3 + CO_2 + HO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G44226 | TrGTerCN | $IPRHOCO3 + NO_2 \rightarrow C4PAN5$ | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G44227 | TrGTerCN | $IPRHOCO3 + NO_3 \rightarrow CH_3COCH_3 + CO_2 + HO_2 + NO_2$ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G44228a | TrGTerC | $IPRHOCO3 \rightarrow CH_3COCH_3 + CO_2 + HO_2$ | k1_R02RC03*0.7 | Rickard and Pascoe (2009) |
| G44228b | TrGTerC | $IPRHOCO3 \rightarrow IPRHOCO2H$ | k1_R02RC03*0.3 | Rickard and Pascoe (2009) |
| G44229 | TrGTerC | $IPRHOCO2H + OH \rightarrow CH_3COCH_3 + CO_2 + HO_2 + H_2O$ | 1.72E-12 | Rickard and Pascoe (2009) |
| G44230 | TrGTerC | $OH + IPRHOCO3H \rightarrow IPRHOCO3$ | 4.80E-12 | Rickard and Pascoe (2009) |
| G44231 | TrGTerCN | $C4PAN5 \rightarrow IPRHOCO3 + NO_2$ | K_PAN_M | Rickard and Pascoe (2009) |
| G44232 | TrGTerCN | $C4PAN5 + OH \rightarrow CH_3COCH_3 + CO + NO_2$ | 4.75E-13 | Rickard and Pascoe (2009) |
| G44233a | TrGTerC | $MBOOO \rightarrow IPRHOCO2H$ | 1.60E-17*C(ind_H20)*(0.08+0.15) | Rickard and Pascoe (2009), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--------------------------|--|
| G44233b | TrGTerC | MBOOO \rightarrow IBUTALOH + H ₂ O ₂ | 1.60E-17*C(ind_H2O)*0.77 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44234 | TrGTerC | MBOOO + CO \rightarrow IBUTALOH + CO ₂ | 1.20E-15 | Rickard and Pascoe (2009) |
| G44235 | TrGTerCN | MBOOO + NO \rightarrow IBUTALOH + NO ₂ | 1.00E-14 | Rickard and Pascoe (2009) |
| G44236 | TrGTerCN | MBOOO + NO ₂ \rightarrow IBUTALOH + NO ₃ | 1.00E-15 | Rickard and Pascoe (2009) |
| G44400 | TrGAroC | MALANHY + OH \rightarrow MALANHYO2 | 1.4E-12 | Rickard and Pascoe (2009) |
| G44401a | TrGAroC | MALDIALOOH + OH \rightarrow HOCOC4DIAL + OH | 1.22E-10 | Rickard and Pascoe (2009) |
| G44401b | TrGAroC | MALDIALOOH + OH \rightarrow MALDIALO2 | 0.6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G44402 | TrGAroCN | NC4DCO2H + OH \rightarrow MALANHY + NO ₂ | 0.6*k_CH300H_OH | Rickard and Pascoe (2009)* |
| G44403 | TrGAroC | CO14O3CO2H + OH \rightarrow HCOCH ₂ O ₂ + 2 CO ₂ | 2.19E-11 | Rickard and Pascoe (2009) |
| G44404 | TrGAroC | BZFUOOH + OH \rightarrow BZFUO2 | 3.68E-11 | Rickard and Pascoe (2009) |
| G44405 | TrGAroC | HOCOC4DIAL + OH \rightarrow CO2C4DIAL + HO ₂ | 3.67E-11 | Rickard and Pascoe (2009) |
| G44406a | TrGAroC | MALDIALCO3 + HO ₂ \rightarrow MALDALCO2H + O ₃ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G44406b | TrGAroC | MALDIALCO3 + HO ₂ \rightarrow MALDALCO3H | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G44406c | TrGAroC | MALDIALCO3 + HO ₂ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009)* |
| G44407 | TrGAroCN | MALDIALCO3 + NO \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂ | KAPNO | Rickard and Pascoe (2009)* |
| G44408 | TrGAroCN | MALDIALCO3 + NO ₂ \rightarrow MALDIALPAN | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G44409 | TrGAroCN | MALDIALCO3 + NO ₃ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009)* |
| G44410 | TrGAroC | MALDIALCO3 \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ | k1_R02RC03 | Rickard and Pascoe (2009)* |
| G44411 | TrGAroCN | BZFUONE + NO ₃ \rightarrow NBZFUO2 | 3.00E-13 | Rickard and Pascoe (2009) |
| G44412 | TrGAroC | BZFUONE + O ₃ \rightarrow .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H ₂ O ₂ + .5 CO + .5 CO ₂ + .5 HCOCH ₂ O ₂ + .5 OH | 2.20E-19 | see note* |
| G44413 | TrGAroC | BZFUONE + OH \rightarrow BZFUO2 | 4.45E-11 | Rickard and Pascoe (2009) |
| G44414 | TrGAroCN | NBZFUOOH + OH \rightarrow NBZFUO2 | 6.18E-12 | Rickard and Pascoe (2009) |
| G44415 | TrGAroC | MALDALCO3H + OH \rightarrow MALDIALCO3 | 4.00E-11 | Rickard and Pascoe (2009) |
| G44416 | TrGAroC | EPXDLCO2H + OH \rightarrow C3DIALO2 + CO ₂ | 2.31E-11 | Rickard and Pascoe (2009) |
| G44417a | TrGAroC | EPXDLCO3 + HO ₂ \rightarrow C3DIALO2 + CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G44417b | TrGAroC | EPXDLCO3 + HO ₂ \rightarrow EPXDLCO2H + O ₃ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G44417c | TrGAroC | EPXDLCO3 + HO ₂ \rightarrow EPXDLCO3H | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G44418 | TrGAroCN | EPXDLCO3 + NO \rightarrow C3DIALO2 + CO ₂ + NO ₂ | KAPNO | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| G44419 | TrGAroCN | EPXDLCO3 + NO ₂ → EPXDLPAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G44420 | TrGAroCN | EPXDLCO3 + NO ₃ → C3DIALO2 + CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G44421 | TrGAroC | EPXDLCO3 → C3DIALO2 + CO ₂ | k1_R02RC03 | 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*KN03AL*2.0 | Rickard and Pascoe (2009) |
| G44424 | TrGAroC | MALDIAL + O ₃ → 1.0675 GLYOX + .125 HCHO + .1125 HCOCO ₂ H + .0675 H ₂ O 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 | KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44429b | TrGAroC | MALANHYO2 + HO ₂ → HCOCOHC03 + CO ₂ + OH | KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44430 | TrGAroCN | MALANHYO2 + NO → HCOCOHC03 + CO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G44431 | TrGAroCN | MALANHYO2 + NO ₃ → HCOCOHC03 + CO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G44432 | TrGAroC | MALANHYO2 → HCOCOHC03 + CO ₂ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G44433 | TrGAroC | EPXDLCO3H + OH → EPXDLCO3 | 2.62E-11 | Rickard and Pascoe (2009) |
| G44434 | TrGAroC | CO2C4DIAL + OH → CO + CO + CO + CO + HO ₂ | 2.45E-11 | Rickard and Pascoe (2009) |
| G44435a | TrGAroCN | NBZFUO2 + HO ₂ → NBZFUOOH | KR02H02(4)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44435b | TrGAroCN | NBZFUO2 + HO ₂ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH | KR02H02(4)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44436 | TrGAroCN | NBZFUO2 + NO → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G44437 | TrGAroCN | NBZFUO2 + NO ₃ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G44438 | TrGAroCN | NBZFUO2 → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ | k1_R02s0R02 | 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*KN03AL*4.0 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|--|
| G44441 | TrGAroC | EPXC4DIAL + OH → EPXDLCO3 | 4.32E-11 | Rickard and Pascoe (2009) |
| G44442a | TrGAroC | MECOACETO2 + HO ₂ → MECOACEOOH | KR02H02(4)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44442b | TrGAroC | MECOACETO2 + HO ₂ → CH ₃ C(O)OO + HCHO + CO ₂ + OH | KR02H02(4)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44443 | TrGAroCN | MECOACETO2 + NO → CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G44444 | TrGAroCN | MECOACETO2 + NO ₃ → CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G44445 | TrGAroC | MECOACETO2 → CH ₃ C(O)OO + HCHO + CO ₂ | k1_R02p0R02 | Rickard and Pascoe (2009)* |
| G44446 | TrGAroCN | CO14O3CHO + NO ₃ → CO + HCOCH ₂ O ₂ + CO ₂ + HNO ₃ | KN03AL*8.0 | Rickard and Pascoe (2009) |
| G44447 | TrGAroC | CO14O3CHO + OH → CO + HCOCH ₂ O 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 | KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44449b | TrGAroC | BZFUO2 + HO ₂ → CO14O3CHO + HO ₂ + OH | KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G44450 | TrGAroCN | BZFUO2 + NO → CO14O3CHO + HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G44451 | TrGAroCN | BZFUO2 + NO ₃ → CO14O3CHO + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G44452 | TrGAroC | BZFUO2 → CO14O3CHO + HO ₂ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G44453 | TrGAroC | BZFUCO + OH → CO14O3CHO + HO ₂ | 1.78E-11 | Rickard and Pascoe (2009) |
| G44456a | TrGAroC | MALDIALO2 + HO ₂ → MALDIALOOH | KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G44456b | TrGAroC | MALDIALO2 + HO ₂ → GLYOX + GLYOX + HO ₂ + OH | KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G44457 | TrGAroCN | MALDIALO2 + NO → GLYOX + GLYOX + HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G44458 | TrGAroCN | MALDIALO2 + NO ₃ → GLYOX + GLYOX + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G44459 | TrGAroC | MALDIALO2 → GLYOX + GLYOX + HO ₂ | k1_R02s0R02 | 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) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|--|
| G45000 | TrGC | $C_5H_8 + O_3 \rightarrow .3508 \text{ MACR} + .01518 \text{ MACO2H} + .2440 \text{ MVK} + .7085 \text{ HCHO} + .11 \text{ CH}_2\text{OO} + .1275 \text{ C}_3\text{H}_6 + .1575 \text{ CH}_3\text{C(O)} + .0510 \text{ CH}_3 + .2625 \text{ HO}_2 + .27 \text{ OH} + .09482 \text{ H}_2\text{O}_2 + .255 \text{ CO}_2 + .522 \text{ CO} + .07182 \text{ HCHO} + .03618 \text{ HCOCH}_2\text{O}_2 + .01782 \text{ CO} + 0.05408 \text{ LCARBON}$ | $1.03E-14 * \text{EXP}(-1995./\text{temp})$ | Atkinson et al. (2006), Taraborrelli (2016) |
| G45001 | TrGC | $C_5H_8 + OH \rightarrow .63 \text{ ISOPAB} + .30 \text{ ISOPCD} + .07 \text{ LISOPEFO2}$ | $2.7E-11 * \text{EXP}(390./\text{temp})$ | Atkinson et al. (2006), Taraborrelli (2016) |
| G45002 | TrGCN | $C_5H_8 + NO_3 \rightarrow \text{NISOP O2}$ | $3.0E-12 * \text{EXP}(-450./\text{temp})$ | Atkinson et al. (2006) |
| G45003a | TrGC | $\text{ISOPAB} + O_2 \rightarrow \text{LISOPACO2}$ | $5.530E-13$ | Taraborrelli (2016) |
| G45003b | TrGC | $\text{ISOPAB} + O_2 \rightarrow \text{ISOPBO2}$ | $3.E-12$ | Taraborrelli (2016) |
| G45004a | TrGC | $\text{ISOPCD} + O_2 \rightarrow \text{LDISOPACO2}$ | $6.780E-13$ | Taraborrelli (2016) |
| G45004b | TrGC | $\text{ISOPCD} + O_2 \rightarrow \text{ISOPDO2}$ | $3.E-12$ | Taraborrelli (2016) |
| G45005 | TrGC | $\text{LISOPACO2} \rightarrow \text{ISOPAB} + O_2$ | $3.1E12 * \text{exp}(-7900./\text{temp}) * .6 + 7.8E13 * \text{exp}(-8600./\text{temp}) * .4$ | Taraborrelli (2016) |
| G45006 | TrGC | $\text{ISOPBO2} \rightarrow \text{ISOPAB} + O_2$ | $3.7E14 * \text{exp}(-9570./\text{temp}) + 4.2E14 * \text{exp}(-9970./\text{temp})$ | Taraborrelli (2016) |
| G45007 | TrGC | $\text{LDISOPACO2} \rightarrow \text{ISOPCD} + O_2$ | $5.65E12 * \text{exp}(-8410./\text{temp}) * .42 + 1.4E14 * \text{exp}(-9110./\text{temp}) * .58$ | Taraborrelli (2016) |
| G45008 | TrGC | $\text{ISOPDO2} \rightarrow \text{ISOPCD} + O_2$ | $5.0E14 * \text{exp}(-10120./\text{temp}) + 8.25E14 * \text{exp}(-10220./\text{temp})$ | Taraborrelli (2016) |
| G45009a | TrGC | $\text{LISOPACO2} \rightarrow \text{C1ODC2O2C4OOH}$ | $K16HSZ14 * 2./3. * (1 - fhpal)$ | Taraborrelli (2016) |
| G45009b | TrGC | $\text{LISOPACO2} \rightarrow \text{ZCODC23DBCOOH} + \text{HO}_2$ | $K16HSZ14 * (2./3. * fhpal + 1./3.)$ | Taraborrelli (2016) |
| G45010a | TrGC | $\text{LDISOPACO2} \rightarrow \text{C1OOHC3O2C4OD}$ | $k16HSZ41 * 2./3. * (1 - fhpal)$ | Taraborrelli (2016) |
| G45010b | TrGC | $\text{LDISOPACO2} \rightarrow \text{ZCODC23DBCOOH} + \text{HO}_2$ | $k16HSZ41 * (2./3. * fhpal + 1./3.)$ | Taraborrelli (2016) |
| G45011 | TrGC | $\text{LISOPACO2} \rightarrow .9 \text{ LISOPACO} + .1 \text{ ISOPA OH}$ | $k1_R02\text{LISOPACO2}$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45012 | TrGC | $\text{LISOPACO2} + \text{HO}_2 \rightarrow \text{LISOPACOOH}$ | $KR02H02(5)$ | Rickard and Pascoe (2009) |
| G45013a | TrGCN | $\text{LISOPACO2} + \text{NO} \rightarrow \text{LISOPACO} + \text{NO}_2$ | $KR02N0 * (1 - \alpha_AN(6, 1, 0, 0, 0, \text{temp}, \text{cair}))$ | Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016) |
| G45013b | TrGCN | $\text{LISOPACO2} + \text{NO} \rightarrow \text{LISOPACNO3}$ | $KR02N0 * \alpha_AN(6, 1, 0, 0, 0, \text{temp}, \text{cair})$ | Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016) |
| G45014 | TrGCN | $\text{LISOPACO2} + \text{NO}_3 \rightarrow \text{LISOPACO} + \text{NO}_2$ | $KR02N03$ | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|--|
| G45015 | TrGC | LDISOPACO2 \rightarrow .9 LISOPACO + .1 ISOPAHOH | k1_R02LISOPACO2 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45016 | TrGC | LDISOPACO2 + HO ₂ \rightarrow LISOPACOOH | KR02H02(5) | Rickard and Pascoe (2009) |
| G45017a | TrGCN | LDISOPACO2 + NO \rightarrow LISOPACO + NO ₂ | KR02N0*(1.-alpha_AN(6,1,0,0,0, temp, cair)) | Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016) |
| G45017b | TrGCN | LDISOPACO2 + NO \rightarrow LISOPACNO3 | KR02N0*alpha_AN(6,1,0,0,0, temp, cair) | Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016) |
| G45018 | TrGCN | LDISOPACO2 + NO ₃ \rightarrow LISOPACO + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G45019a | TrGC | LISOPACOOH + OH \rightarrow LISOPACO2 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45019b | TrGC | LISOPACOOH + OH \rightarrow ZCODC23DBCOOH + HO ₂ | k_s*f_allyl*f_soh | Taraborrelli (2016) |
| G45019c | TrGC | LISOPACOOH + OH \rightarrow LHC4ACCHO + OH | (k_s*f_soh*f_allyl+ k_rohro) | Taraborrelli (2016) |
| G45019d | TrGC | LISOPACOOH + OH \rightarrow LIEPOX + OH | (k_adt+k_ads)*a_ch2oh*a_ch2ooh | Taraborrelli (2016)* |
| G45020 | TrGC | ISOPAHOH + OH \rightarrow LHC4ACCHO + HO ₂ | (k_adt+k_ads)*a_ch2oh*a_ch2oh+k_s*f_soh*f_allyl+k_rohro | Taraborrelli (2016) |
| G45021 | TrGCN | LISOPACNO3 + OH \rightarrow LISOPACNO3O2 | (k_adt+k_ads)*a_ch2ono2*a_ch2oh | Taraborrelli (2016)* |
| G45022 | TrGC | ISOPBO2 \rightarrow .8 MVK + .8 HCHO + .8 HO ₂ + .2 ISOPBOH | k1_R02ISOPBO2 | Rickard and Pascoe (2009) |
| G45023a | TrGC | ISOPBO2 + HO ₂ \rightarrow ISOPBOOH | KR02H02(5)*(1.-rchohch2o2_oh) | Taraborrelli (2016) |
| G45023b | TrGC | ISOPBO2 + HO ₂ \rightarrow MVK + HCHO + HO ₂ + OH | KR02H02(5)*rchohch2o2_oh | Taraborrelli (2016) |
| G45024a | TrGCN | ISOPBO2 + NO \rightarrow MVK + HCHO + HO ₂ + NO ₂ | KR02N0*(1.-alpha_AN(6,3,0,0,0, temp, cair)) | Lockwood et al. (2010), Taraborrelli (2016) |
| G45024b | TrGCN | ISOPBO2 + NO \rightarrow ISOPBNO3 | KR02N0*alpha_AN(6,3,0,0,0, temp, cair) | Lockwood et al. (2010), Taraborrelli (2016) |
| G45025 | TrGCN | ISOPBO2 + NO ₃ \rightarrow MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃ + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G45026a | TrGC | ISOPBOOH + OH \rightarrow LIEPOX + OH | (k_ads+k_adp)*a_ch2ooh | Paulot et al. (2009b), Taraborrelli (2016) |
| G45026b | TrGC | ISOPBOOH + OH \rightarrow ISOPBO2 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45026c | TrGC | ISOPBOOH + OH \rightarrow MGLYOX + HOCH ₂ CHO | k_rohro+k_s*f_alk*f_soh | Taraborrelli (2016) |
| G45027 | TrGC | ISOPBOOH + O ₃ \rightarrow .1368 MACROOH + .1368 H ₂ O ₂ + .2280 HO ₂ + .4332 CH ₃ COCH ₂ OH + .2280 CO ₂ + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO ₂ + .06880 OH + .2709 CO + .1591 CH ₂ OO | 1.E-17 | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|---|
| 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 | Taraborrelli (2016) |
| G45029 | TrGCN | ISOPBNO ₃ + OH → ISOPBDNO ₃ O ₂ | (k_adt+k_adp)*f_ch2ono2 | Taraborrelli (2016) |
| G45030 | TrGC | ISOPDO ₂ → .8 MACR + .8 HCHO + .8 HO ₂ + .1 HCOC ₅ + .1 ISOPDOH | k1_R02ISOPD02 | Rickard and Pascoe (2009) |
| G45031a | TrGC | ISOPDO ₂ + HO ₂ → ISOPDOOH | KR02H02(5)*(1.-rchohch2o2_oh) | Taraborrelli (2016) |
| G45031b | TrGC | ISOPDO ₂ + HO ₂ → MACR + HCHO + HO ₂ + OH | KR02H02(5)*rchohch2o2_oh | Taraborrelli (2016) |
| G45032a | TrGCN | ISOPDO ₂ + NO → MACR + HCHO + HO ₂ + NO ₂ | KR02N0*(1.-alpha_AN(6,2,0,0,0,temp,cair)) | Lockwood et al. (2010), Taraborrelli (2016) |
| G45032b | TrGCN | ISOPDO ₂ + NO → ISOPDNO ₃ | KR02N0*alpha_AN(6,2,0,0,0,temp,cair) | Lockwood et al. (2010), Taraborrelli (2016) |
| G45033 | TrGCN | ISOPDO ₂ + NO ₃ → MACR + HCHO + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G45034a | TrGC | ISOPDOOH + OH → LIEPOX + OH | (k_adt+k_adp)*a_ch2ooh | Paulot et al. (2009b), Taraborrelli (2016) |
| G45034b | TrGC | ISOPDOOH + OH → ISOPDO ₂ | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45034c | TrGC | ISOPDOOH + OH → HCOC ₅ + OH | k_t*f_tooh*f_allyl*f_pch2oh | Taraborrelli (2016) |
| G45034d | TrGC | ISOPDOOH + OH → CH ₃ COCH ₂ OH + GLYOX + OH | k_s*f_pch2oh*f_soh | Taraborrelli (2016) |
| G45035 | TrGC | ISOPDOOH + O ₃ → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO ₂ + .2079 CO + .1221 CH ₂ OO | 1.E-17 | Taraborrelli (2016) |
| G45036 | TrGC | ISOPDOH + OH → HCOC ₅ + HO ₂ | 2.*k_rohro+(k_t*f_toh*f_allyl+k_s*f_soh)*f_pch2oh+(k_adt+k_adp)*a_ch2oh | Taraborrelli (2016) |
| G45037 | TrGCN | ISOPDNO ₃ + OH → ISOPBDNO ₃ O ₂ | (k_adp+k_ads)*a_ch2ono2 | Taraborrelli (2016)* |
| G45038 | TrGCN | NISOPO ₂ → .8 NC ₄ CHO + .6 HO ₂ + .2 LISOPACNO ₃ | k1_R02LISOPAC02 | Rickard and Pascoe (2009) |
| G45039 | TrGCN | NISOPO ₂ + HO ₂ → NISOPOOH | KR02H02(5) | Rickard and Pascoe (2009) |
| G45040 | TrGCN | NISOPO ₂ + NO → NC ₄ CHO + HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G45041 | TrGCN | NISOPO ₂ + NO ₃ → NC ₄ CHO + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G45042 | TrGCN | NISOPOOH + OH → NC ₄ CHO + OH | 1.03E-10 | Rickard and Pascoe (2009) |
| G45043 | TrGCN | NC ₄ CHO + OH → LNISO ₃ | (k_adt+k_ads)*a_cho*a_ch2ono2 | Taraborrelli (2016)* |
| G45044 | TrGCN | NC ₄ CHO + O ₃ → .27 NOA + .027 HCOCO ₂ H + .0162 GLYOX + .0162 H ₂ O 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 | Taraborrelli (2016) |
| G45045 | TrGCN | NC ₄ CHO + NO ₃ → LNISO ₃ + HNO ₃ | KN03AL*4.25 | Rickard and Pascoe (2009) |
| G45046 | TrGCN | LNISO ₃ + HO ₂ → LNISOOH | .5*KR02H02(5) + .5*KAPH02 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|----------------------------|
| G45047 | TrGCN | LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂ | .5*KAPNO +.5*KR02NO | Rickard and Pascoe (2009)* |
| G45048 | TrGCN | LNISO3 + NO ₃ → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂ | 1.3*KR02NO3 | 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 | Taraborrelli (2016) |
| G45050b | TrGC | LHC4ACCHO + OH → LHC4ACCO3 | k_t*f_o | Taraborrelli (2016) |
| G45050c | TrGC | LHC4ACCHO + OH → ZCODC23DBCOD + HO ₂ | k_s*f_soh*f_allyl | Taraborrelli (2016) |
| G45051 | TrGC | LHC4ACCHO + O ₃ → .2225 CH ₃ C(O) + .89 CO + .0171875 HOCH ₂ CO ₂ H + .075625 H ₂ O ₂ + .0171875 HCOCO ₂ H + .2775 CH ₃ COCH ₂ OH + .6675 HO ₂ + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 HOCH ₂ CHO + .5 MGLYOX | 2.40E-17 | Rickard and Pascoe (2009) |
| G45052 | TrGCN | LHC4ACCHO + NO ₃ → LHC4ACCO3 + HNO ₃ | KN03AL*4.25 | Rickard and Pascoe (2009) |
| G45053 | TrGC | LC578O2 → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ | k1_R02t0R02 | Rickard and Pascoe (2009) |
| G45054a | TrGC | LC578O2 + HO ₂ → MGLYOX + HOCH ₂ CHO + OH | KR02H02(5)*rcoch2o2_oh | Rickard and Pascoe (2009) |
| G45054b | TrGC | LC578O2 + HO ₂ → LC578OOH | KR02H02(5)*rcoch2o2_ohh | Rickard and Pascoe (2009) |
| G45055 | TrGCN | LC578O2 + NO → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |
| G45056 | TrGCN | LC578O2 + NO ₃ → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ + NO ₂ | KR02NO3 | Rickard and Pascoe (2009) |
| G45057 | TrGC | LC578O2 → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCH ₂ CHO + .75 HOCH ₂ CHO + HO ₂ + OH | KHSB | Taraborrelli (2016) |
| G45058a | TrGC | LC578OOH + OH → LC578O2 | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45058b | TrGC | LC578OOH + OH → C10DC20OHC4OD + HO ₂ | k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_pch2oh*f_pch2oh+k_s*f_soh*f_pch2oh | Taraborrelli (2016) |
| G45059a | TrGC | LHC4ACCO3 → OH + .5 MACRO2 + .5 LHMVKABO2 + CO ₂ | k1_R02RC03*0.9 | Taraborrelli (2016) |
| G45059b | TrGC | LHC4ACCO3 → LHC4ACCO2H | k1_R02RC03*0.1 | Taraborrelli (2016) |
| G45060a | TrGC | LHC4ACCO3 + HO ₂ → 2 OH + .5 MACRO2 + .5 LHMVKABO2 + CO ₂ | KAPH02*rco3_oh | Taraborrelli (2016) |
| G45060b | TrGC | LHC4ACCO3 + HO ₂ → LHC4ACCO3H | KAPH02*rco3_ohh | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|---|--|
| G45060c | TrGC | $\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$ | KAPH02*rco3_o3 | Taraborrelli (2016) |
| G45061 | TrGCN | $\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$ | KAPNO | Taraborrelli (2016) |
| G45062 | TrGCN | $\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45063 | TrGCN | $\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$ | 1.6*KR02N03 | Taraborrelli (2016) |
| G45064a | TrGC | $\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$ | 2.52E-11 | Taraborrelli (2016) |
| G45064b | TrGC | $\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$ | 2.88E-11 | Rickard and Pascoe (2009) |
| G45065 | TrGCN | $\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45066 | TrGCN | $\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$ | 2.52E-11 | Rickard and Pascoe (2009) |
| G45067 | TrGC | $\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$ | 3.81E-11 | Rickard and Pascoe (2009) |
| G45068 | TrGC | $\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{ H}_2\text{O}_2 + .67 \text{ HCHO} + .2079 \text{ CO} + .1221 \text{ CH}_2\text{OO} + .05280 \text{ OH}$ | $7.51\text{E-}16*\text{EXP}(-1521./\text{temp})$ | Taraborrelli (2016) |
| G45069 | TrGC | $\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$ | k1_R02t0R02 | Taraborrelli (2016) |
| G45070a | TrGC | $\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$ | KR02H02(5)*rcoch2o2_oh | Taraborrelli (2016) |
| G45070b | TrGC | $\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$ | KR02H02(5)*rcoch2o2_ooh | Taraborrelli (2016) |
| G45071 | TrGCN | $\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G45072 | TrGCN | $\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G45073 | TrGC | $\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$ | 9.7E-12 | Rickard and Pascoe (2009) |
| G45074 | TrGC | $\text{LIEPOX} + \text{OH} \rightarrow \text{DB1O2} + \text{H}_2\text{O}$ | $5.78\text{E-}11*\text{EXP}(-400./\text{temp}) * (1.52/3.+0.98*2./3.)/1.51$ | Paulot et al. (2009b), Bates et al. (2014), Taraborrelli (2016)* |
| G45075 | TrGC | $\text{ISOPBO2} \rightarrow \text{MVK} + \text{HCHO} + \text{OH}$ | KHSB | Taraborrelli (2016) |
| G45076 | TrGC | $\text{ISOPDO2} \rightarrow \text{MACR} + \text{HCHO} + \text{OH}$ | KHSD | Taraborrelli (2016) |
| G45077a | TrGC | $\text{ZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC2O2C4OOH} + .4 \text{ C1OOHC2O2C4OD}$ | k_adt*a_cho*a_ch2ooh | Taraborrelli (2016) |
| G45077b | TrGC | $\text{ZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC3O2C4OOH} + .4 \text{ C1OOHC3O2C4OD}$ | k_ads*a_cho*a_ch2ooh | Taraborrelli (2016) |
| G45077c | TrGC | $\text{ZCODC23DBCOOH} + \text{OH} \rightarrow \text{ZCO3HC23DBCOD}$ | k_t*f_o*f_alk+0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45077d | TrGC | $\text{ZCODC23DBCOOH} + \text{OH} \rightarrow \text{ZCODC23DBCOD} + \text{OH}$ | k_s*f_sooh*f_allyl | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|----------------------|
| G45078 | TrGC | ZCODC23DBCOOH + O ₃ → .4672 OH + .2336 HCOCOCH ₂ O ₂ + .2336 CO + .2336 CH ₃ C(O) + .4672 HOOCH ₂ CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH ₂ CHO + .02765 H ₂ O ₂ + .02592 CH ₃ OOH + .02592 CO ₂ + .01037 HCOCO + .01555 CH ₂ OO + .01555 CO + .006908 HOOCH ₂ CO ₃ + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH ₂ OOH + .2628 GLYOX + .0972 CH ₃ COCH ₂ O ₂ H + .00972 HCOCO ₂ H + .005832 GLYOX + .005832 H ₂ O ₂ + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO ₂ + .01458 HCOOH + .01458 CO | 2.4E-17 | Taraborrelli (2016) |
| G45079 | TrGC | C1OOHC2O2C4OD → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH | k1_R02t0R02 | Taraborrelli (2016) |
| G45080 | TrGCN | C1OOHC2O2C4OD + NO → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH + NO ₂ | KR02N0 | Taraborrelli (2016)* |
| G45081a | TrGC | C1OOHC2O2C4OD + HO ₂ → C1OOHC2OOHC4OD | KR02H02(5)*rcoch2o2_ooH | Taraborrelli (2016) |
| G45081b | TrGC | C1OOHC2O2C4OD + HO ₂ → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + 1.22 OH | KR02H02(5)*rcoch2o2_oh | Taraborrelli (2016) |
| G45082 | TrGC | C1OOHC2O2C4OD → CH ₃ COCH ₂ O ₂ H + GLYOX + OH | KHSB | Taraborrelli (2016) |
| G45083 | TrGC | C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD | K15HSDHB | Taraborrelli (2016) |
| G45084a | TrGC | C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH | 2.*k_s*f_sooh*f_tch2oh | Taraborrelli (2016) |
| G45084b | TrGC | C1OOHC2OOHC4OD + OH → CH ₃ COCH ₂ O ₂ H + 2 CO + 2 HO ₂ + OH | k_t*f_toh*f_pch2oh*f_pch2oh | Taraborrelli (2016) |
| G45084c | TrGC | C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD | 0.6*k_CH300H_OH | Taraborrelli (2016) |
| G45085 | TrGC | C1ODC2OOHC4OD + OH → CO ₂ H ₃ CHO + CO + H ₂ O + OH | k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho | Taraborrelli (2016) |
| G45086 | TrGC | C1ODC3O2C4OOH → MGLYOX + HOOCH ₂ CHO + HO ₂ | k1_R02s0R02 | Taraborrelli (2016) |
| G45087 | TrGCN | C1ODC3O2C4OOH + NO → MGLYOX + HOOCH ₂ CHO + HO ₂ + NO ₂ | KR02N0 | Taraborrelli (2016) |
| G45088 | TrGC | C1ODC3O2C4OOH + HO ₂ → .5 CH ₃ C(O) + .5 CO + .5 MGLYOX + .5 HO ₂ + HOOCH ₂ CO ₃ | KR02H02(5) | Taraborrelli (2016) |
| G45089 | TrGC | C1ODC3O2C4OOH → MGLYOX + OH + HOOCH ₂ CHO | KHSD | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|--|--|
| G45090 | TrGC | $C10OHC3O2C4OD \rightarrow .625 \text{ MGLYOX} + 2 \text{ CO} + 1.625 \text{ HO}_2 + .375 \text{ CH}_3\text{C(O)} + .375 \text{ CO}_2 + \text{ OH}$ | K15HSDHB | Taraborrelli (2016) |
| G45091 | TrGC | $\text{LHC4ACCO}_3 \rightarrow \text{ZCO}_3\text{HC}_2\text{3DBCOD} + \text{HO}_2$ | K16HS | Taraborrelli (2016) |
| G45092a | TrGC | $\text{ZCODC}_2\text{3DBCOD} + \text{OH} \rightarrow \text{C1ODC}_2\text{O}_2\text{C}_4\text{OD}$ | $(k_{\text{adt}}+k_{\text{ads}})*a_{\text{cho}}*a_{\text{cho}}$ | Taraborrelli (2016)* |
| G45092b | TrGC | $\text{ZCODC}_2\text{3DBCOD} + \text{OH} \rightarrow \text{ZCO}_3\text{C}_2\text{3DBCOD}$ | $2*k_{\text{t}}*f_{\text{o}}*f_{\text{alk}}$ | Taraborrelli (2016)* |
| G45093 | TrGCN | $\text{ZCODC}_2\text{3DBCOD} + \text{NO}_3 \rightarrow \text{ZCO}_3\text{C}_2\text{3DBCOD} + \text{HNO}_3$ | $\text{KN03AL}*4.25*2.$ | Taraborrelli (2016)* |
| G45094a | TrGC | $\text{C1ODC}_2\text{O}_2\text{C}_4\text{OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$ | $\text{KR02H02(5)}*r_{\text{coch2o2_oh}}$ | Taraborrelli (2016) |
| G45094b | TrGC | $\text{C1ODC}_2\text{O}_2\text{C}_4\text{OD} + \text{HO}_2 \rightarrow \text{C1ODC}_2\text{OOHC}_4\text{OD}$ | $\text{KR02H02(5)}*r_{\text{coch2o2_ooh}}$ | Taraborrelli (2016) |
| G45095 | TrGCN | $\text{C1ODC}_2\text{O}_2\text{C}_4\text{OD} + \text{NO} \rightarrow \text{NO}_2 + \text{MGLYOX} + \text{HOCHCHO}$ | KR02N0 | Taraborrelli (2016)* |
| G45096 | TrGC | $\text{C1ODC}_2\text{O}_2\text{C}_4\text{OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$ | $k1_{\text{R02t0R02}}$ | Taraborrelli (2016) |
| G45097a | TrGC | $\text{C1ODC}_2\text{OOHC}_4\text{OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO}$ | $(2*k_{\text{t}}*f_{\text{o}}*f_{\text{tch2oh}}*f_{\text{alk}}+k_{\text{t}}*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$ | Taraborrelli (2016) |
| G45097b | TrGC | $\text{C1ODC}_2\text{OOHC}_4\text{OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + \text{OH}$ | $(2*k_{\text{t}}*f_{\text{o}}*f_{\text{tch2oh}}*f_{\text{alk}}+k_{\text{t}}*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$ | Taraborrelli (2016) |
| G45098 | TrGCN | $\text{LISOPACNO}_3\text{O}_2 + \text{NO} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO}_2\text{CO}_3\text{C}_4 + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO}_3 + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2 + \text{NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G45099 | TrGCN | $\text{LISOPACNO}_3\text{O}_2 \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO}_2\text{CO}_3\text{C}_4 + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO}_3 + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2$ | $k1_{\text{R02t0R02}}+\text{KR02H02(5)}*c(\text{ind}_{\text{H02}})$ | Taraborrelli (2016) |
| G45100 | TrGCN | $\text{ISOPBDNO}_3\text{O}_2 + \text{NO} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRN} + .14 \text{ MVKNO}_3 + .4 \text{ HCHO} + .4 \text{ HO}_2 + 1.6 \text{ NO}_2$ | KR02N0 | Taraborrelli (2016)* |
| G45101 | TrGCN | $\text{ISOPBDNO}_3\text{O}_2 \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRN} + .14 \text{ MVKNO}_3 + .4 \text{ HCHO} + .4 \text{ HO}_2 + .6 \text{ NO}_2$ | $k1_{\text{R02s0R02}}+\text{KR02H02(5)}*c(\text{ind}_{\text{H02}})$ | Taraborrelli (2016) |
| G45102 | TrGCN | $\text{LISOPACNO}_3 + \text{O}_3 \rightarrow .8704 \text{ OH} + .365 \text{ HO}_2 + .73 \text{ MGLYOX} + .4325 \text{ NO}_3\text{CH}_2\text{CHO} + .135 \text{ CH}_3\text{COCH}_2\text{OH} + .0675 \text{ GLYOX} + .4325 \text{ NO}_2 + .0891 \text{ H}_2\text{O}_2 + .135 \text{ NOA} + .0675 \text{ HOCHCHO} + .3866 \text{ HOCH}_2\text{CHO} + .0405 \text{ CH}_3\text{OH} + .0405 \text{ CO} + .0054 \text{ HOCH}_2\text{CO}$ | $2.8\text{E}-17$ | Feierabend et al. (2008), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|---|---|--------------------------------------|
| G45103 | TrGC | DB1O2 → DB1O2 | k1_R02s0R02 | Taraborrelli (2016) |
| G45104a | TrGC | DB1O2 + HO ₂ → DB1OOH | KR02H02(5)*(1.-rchohch2o2_oh) | Taraborrelli (2016)* |
| G45104b | TrGC | DB1O2 + HO ₂ → DB1O2 + OH | KR02H02(5)*rchohch2o2_oh | Taraborrelli (2016) |
| G45105a | TrGCN | DB1O2 + NO → DB1O2 + NO ₂ | KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair)) | Taraborrelli (2016) |
| G45105b | TrGCN | DB1O2 + NO → DB1NO3 | KR02N0*alpha_AN(7,2,0,0,0,temp, cair) | Taraborrelli (2016) |
| G45106 | TrGCN | DB1O2 + NO ₃ → DB1O2 + NO ₂ | KR02N03 | Taraborrelli (2016) |
| 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 ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ | k1_R02s0R02 | Taraborrelli (2016) |
| G45110a | TrGC | DB1O2 + HO ₂ → DB2OOH | KR02H02(5)*(1.-rchohch2o2_oh) | Taraborrelli (2016) |
| G45110b | TrGC | DB1O2 + HO ₂ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH | KR02H02(5)*rchohch2o2_oh | Taraborrelli (2016) |
| G45111 | TrGCN | DB1O2 + NO → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂ | KR02N0 | see note* |
| G45112 | TrGCN | DB1O2 + NO ₃ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂ | KR02N03 | Taraborrelli (2016) |
| G45113 | TrGC | DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH | K14HSAL | Taraborrelli (2016) |
| G45114a | TrGC | DB1OOH + OH → DB1O2 | .6*k_CH300H_OH | Taraborrelli (2016) |
| G45114b | TrGC | DB1OOH + OH → HCOOH + HO ₂ + CH ₃ COCHO ₂ CHO | k_adt | Taraborrelli (2016)* |
| G45115 | TrGC | DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH | 4.67E-26*temp**3.286*EXP(4509./ (1.987*temp)) | Taraborrelli (2016), daSilva (2010)* |
| G45116 | TrGCN | DB1NO3 + OH → HCOOH + NO ₂ + CH ₃ COCHO ₂ CHO | k_adt | Taraborrelli (2016)* |
| G45117 | TrGC | DB2OOH + OH → DB1O2 | .6*k_CH300H_OH | Taraborrelli (2016)* |
| G45118 | TrGC | LISOPACOOH + O ₃ → 1.3272 OH + .36986 HO ₂ + .0432 H ₂ O ₂ + .08422 CO + .2025 CH ₃ OOH + .01215 CH ₂ OO + .3704 HCHO + .00405 CH ₃ OH + .0405 CO ₂ + .1825 HOCH ₂ COCH ₂ O ₂ + .365 MGLYOX + .3866 HOOCH ₂ CHO + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .00324 HCOCO + .3866 HOCH ₂ CHO + .135 CH ₃ COCH ₂ O ₂ H + .0675 HOCHCHO + .0054 HOCH ₂ CO | 4.829E-16 | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|--------|--|--|---|
| G45119a | TrGC | $\text{ZCO3HC23DBCOD} + \text{OH} \rightarrow .62 \text{ CO2H3CHO} + .62 \text{ OH} + .62 \text{ CO}_2 + .38 \text{ MGLYOX} + .38 \text{ HCOCO}_3\text{H} + .38 \text{ HO}_2$ | $k_{\text{adt}}*a_{\text{cho}}*a_{\text{co2h}}$ | Taraborrelli (2016) |
| G45119b | TrGC | $\text{ZCO3HC23DBCOD} + \text{OH} \rightarrow .62 \text{ CH}_3\text{COCO}_3\text{H} + 1.24 \text{ CO} + 1.24 \text{ HO}_2 + .38 \text{ MGLYOX} + .38 \text{ HO}_2 + .38 \text{ CO} + .38 \text{ HO}_2 + .38 \text{ OH} + .38 \text{ CO}_2$ | $k_{\text{ads}}*a_{\text{cho}}*a_{\text{co2h}}$ | Taraborrelli (2016) |
| G45120 | TrGC | $\text{LISOPEFO2} \rightarrow \text{LISOPEFO}$ | $k1_{\text{R02p0R02}}$ | Taraborrelli (2016) |
| G45121a | TrGCN | $\text{LISOPEFO2} + \text{NO} \rightarrow \text{LISOPEFO} + \text{NO}_2$ | $\text{KR02N0}*(1.-\alpha_{\text{AN}}(6,1,0,0,0, \text{temp}, \text{cair}))$ | Taraborrelli (2016) |
| G45121b | TrGCN | $\text{LISOPEFO2} + \text{NO} \rightarrow \text{ISOPDNO3}$ | $\text{KR02N0}*\alpha_{\text{AN}}(6,1,0,0,0, \text{temp}, \text{cair})$ | Taraborrelli (2016)* |
| G45122a | TrGC | $\text{LISOPEFO2} + \text{HO}_2 \rightarrow .7143 \text{ ISOPDOOH} + .2857 \text{ ISOPBOOH}$ | $\text{KR02H02}(5)*(1.-\text{rchohch2o2}_{\text{oh}})$ | Taraborrelli (2016) |
| G45122b | TrGC | $\text{LISOPEFO2} + \text{HO}_2 \rightarrow \text{LISOPEFO} + \text{OH}$ | $\text{KR02H02}(5)*\text{rchohch2o2}_{\text{oh}}$ | Taraborrelli (2016) |
| G45123 | TrGCN | $\text{LISOPEFO2} + \text{NO}_3 \rightarrow \text{LISOPEFO} + \text{NO}_2$ | KR02N03 | Taraborrelli (2016) |
| G45124 | TrGC | $\text{LISOPEFO2} \rightarrow .7143 \text{ MACR} + .2857 \text{ MVK} + \text{HCHO} + \text{OH}$ | $.7143*\text{KHSD}+.2857*\text{KHSB}$ | Taraborrelli (2016) |
| G45125 | TrGC | $\text{LISOPEFO} \rightarrow .7143 \text{ MACR} + .2857 \text{ MVK} + \text{HCHO} + \text{HO}_2$ | KDEC | Taraborrelli (2016) |
| G45126a | TrGC | $\text{LISOPACO} \rightarrow 3\text{METHYLFURAN} + \text{HO}_2$ | $\text{KDEC}*0.37$ | Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45126b | TrGC | $\text{LISOPACO} \rightarrow .65 \text{ LHC4ACCHO} + .65 \text{ HO}_2 + .35 \text{ DB1O2}$ | $\text{KDEC}*(1.-0.37)$ | Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45127a | TrGC | $\text{LISOPACO} \rightarrow 3\text{METHYLFURAN} + \text{HO}_2$ | $\text{KDEC}*0.37$ | Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45127b | TrGC | $\text{LISOPACO} \rightarrow .65 \text{ LHC4ACCHO} + .65 \text{ HO}_2 + .35 \text{ DB1O2}$ | $\text{KDEC}*(1.-0.37)$ | Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003) |
| G45128 | TrGC | $3\text{METHYLFURAN} + \text{OH} \rightarrow \text{L3METHYLFURANO2}$ | $3.2\text{E}-11*\text{EXP}(310./\text{temp})$ | Taraborrelli (2016)* |
| G45129 | TrGCN | $3\text{METHYLFURAN} + \text{NO}_3 \rightarrow \text{L3METHYLFURANO2} + \text{NO}_2$ | $1.9\text{E}-11$ | Taraborrelli (2016), Atkinson et al. (2006)* |
| G45130 | TrGC | $\text{L3METHYLFURANO2} \rightarrow \text{ZCODC23DBCOD} + \text{HO}_2$ | $k1_{\text{R02s0R02}}$ | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---------------------------|--|
| G45131 | TrGCN | L3METHYLFURANO2 + NO → ZCODC23DBCOD + HO ₂ + NO ₂ | KR02N0 | Taraborrelli (2016)* |
| G45132 | TrGC | L3METHYLFURANO2 + HO ₂ → ZCODC23DBCOD + HO ₂ | KR02H02(5) | Taraborrelli (2016)* |
| G45133 | TrGC | ZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ | k1_R02RC03 | Taraborrelli (2016) |
| G45134a | TrGC | ZCO3C23DBCOD + HO ₂ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH | KAPH02*rco3_oh | Taraborrelli (2016) |
| G45134b | TrGC | ZCO3C23DBCOD + HO ₂ → ZCO3HC23DBCOD | KAPH02*(rco3_ooh+rco3_o3) | Taraborrelli (2016)* |
| G45135 | TrGCN | ZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂ | KAPN0 | Taraborrelli (2016) |
| G45136 | TrGCN | ZCO3C23DBCOD + NO ₂ → ZCPANC23DBCOD | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G45137 | TrGCN | ZCO3C23DBCOD + NO ₃ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂ | 1.6*KR02N03 | Taraborrelli (2016) |
| G45138 | TrGCN | ZCPANC23DBCOD → ZCO3C23DBCOD + NO ₂ | k_PAN_M | Rickard and Pascoe (2009) |
| G45139 | TrGCN | ZCPANC23DBCOD + OH → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂ | 2.52E-11 | Taraborrelli (2016)* |
| G45200 | TrGTerC | C511O2 → CH ₃ C(O) + HCOCH2CHO | k1_R02s0R02 | Rickard and Pascoe (2009) |
| G45201 | TrGTerCN | C511O2 + NO → CH ₃ C(O) + HCOCH2CHO + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G45202a | TrGTerC | C511O2 + HO ₂ → C511OOH | KR02H02(5)*rcoch2o2_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45202b | TrGTerC | C511O2 + HO ₂ → CH ₃ C(O) + HCOCH2CHO + OH | KR02H02(5)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| 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 | KN03AL*5.5 | Rickard and Pascoe (2009) |
| G45206 | TrGTerC | CO23C4CO3 → CH ₃ COCOCH ₂ O ₂ + CO ₂ | k1_R02RC03 | Rickard and Pascoe (2009) |
| G45207 | TrGTerCN | CO23C4CO3 + NO → CH ₃ COCOCH ₂ O ₂ + CO ₂ + NO ₂ | KAPN0 | Rickard and Pascoe (2009)* |
| G45208 | TrGTerCN | CO23C4CO3 + NO ₂ → C5PAN9 | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G45209a | TrGTerC | CO23C4CO3 + HO ₂ → CO23C4CO3H | KAPH02*(rco3_ooh+rco3_o3) | Rickard and Pascoe (2009) |
| G45209b | TrGTerC | CO23C4CO3 + HO ₂ → CH ₃ COCOCH ₂ O ₂ + CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G45210 | TrGTerCN | C5PAN9 → CO23C4CO3 + NO ₂ | k_PAN_M | Rickard and Pascoe (2009) |
| G45211 | TrGTerCN | C5PAN9 + OH → CH ₃ COCOCHO + CO + NO ₂ | 3.12E-13 | Rickard and Pascoe (2009) |
| G45212 | TrGTerC | C512O2 → C513O2 | k1_R02pR02 | Rickard and Pascoe (2009) |
| G45213 | TrGTerC | C512O2 + HO ₂ → C512OOH | KR02H02(5) | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|--|
| G45214 | TrGTerCN | $C512O2 + NO \rightarrow C513O2 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G45215 | TrGTerC | $C512OOH + OH \rightarrow CO13C4CHO + OH$ | 1.01E-10 | Rickard and Pascoe (2009) |
| G45216 | TrGTerC | $C513O2 \rightarrow GLYOX + HOC_2H_4CO_3$ | k1_R02sR02 | Rickard and Pascoe (2009) |
| G45217 | TrGTerCN | $C513O2 + NO \rightarrow GLYOX + HOC_2H_4CO_3 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G45218a | TrGTerC | $C513O2 + HO_2 \rightarrow C513OOH$ | KR02H02(5)*rcoch2o2_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45218b | TrGTerC | $C513O2 + HO_2 \rightarrow GLYOX + HOC_2H_4CO_3 + OH$ | KR02H02(5)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45219 | TrGTerC | $CO13C4CHO + OH \rightarrow CHOC3COCO3$ | 1.33E-10 | Rickard and Pascoe (2009) |
| G45220 | TrGTerCN | $CO13C4CHO + NO_3 \rightarrow CHOC3COCO3 + HNO_3$ | 2.*KN03AL*5.5 | Rickard and Pascoe (2009) |
| G45221 | TrGTerC | $C513OOH + OH \rightarrow C513CO + OH$ | 9.23E-11 | Rickard and Pascoe (2009) |
| G45222 | TrGTerC | $CHOC3COCO3 \rightarrow CHOC3COO2 + CO_2$ | k1_R02RCO3 | Rickard and Pascoe (2009) |
| G45223 | TrGTerC | $CHOC3COCO3 + HO_2 \rightarrow CHOC3COOOH$ | KAPH02 | Rickard and Pascoe (2009) |
| G45224 | TrGTerCN | $CHOC3COCO3 + NO_2 \rightarrow CHOC3COPAN$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G45225 | TrGTerCN | $CHOC3COCO3 + NO \rightarrow CHOC3COO2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G45226 | TrGTerC | $C513CO + OH \rightarrow HOC_2H_4CO_3 + CO + CO$ | 2.64E-11 | Rickard and Pascoe (2009) |
| G45227 | TrGTerC | $C514O2 + HO_2 \rightarrow C514OOH$ | KR02H02(5) | Rickard and Pascoe (2009) |
| G45228a | TrGTerCN | $C514O2 + NO \rightarrow CO13C4CHO + HO_2 + NO_2$ | KR02NO*(1.-alpha_AN(7,2,0,1,0, temp,cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45228b | TrGTerCN | $C514O2 + NO \rightarrow C514NO3$ | KR02NO*alpha_AN(7,2,0,1,0,temp, cair) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45229 | TrGTerCN | $C514O2 + NO_3 \rightarrow CO13C4CHO + HO_2 + NO_2$ | KR02NO3 | Rickard and Pascoe (2009) |
| G45230 | TrGTerC | $C514O2 \rightarrow CO13C4CHO + HO_2$ | k1_R02sR02 | Rickard and Pascoe (2009) |
| G45231 | TrGTerC | $C514OOH + OH \rightarrow CO13C4CHO + OH$ | 1.10E-10 | Rickard and Pascoe (2009) |
| G45232 | TrGTerCN | $C514NO3 + OH \rightarrow CO13C4CHO + NO_2$ | 4.33E-11 | Rickard and Pascoe (2009) |
| G45233 | TrGTerC | $CHOC3COOOH + OH \rightarrow CHOC3COCO3$ | 7.55E-11 | Rickard and Pascoe (2009) |
| G45234 | TrGTerCN | $CHOC3COPAN \rightarrow CHOC3COCO3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G45235 | TrGTerCN | $CHOC3COPAN + OH \rightarrow C4CODIAL + CO + NO_2$ | 7.19E-11 | Rickard and Pascoe (2009) |
| G45236 | TrGTerC | $MBO + OH \rightarrow LMBOABO2$ | 8.1E-12*EXP(610./TEMP) | Rickard and Pascoe (2009), Taraborrelli (2016)* |
| G45237a | TrGTerC | $MBO + O_3 \rightarrow HCHO + .16 CH_3COCH_3 + .16 HO_2 + .16 CO + .16 OH + .84 MBOOO$ | 1.0E-17*0.57 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45237b | TrGTerC | $MBO + O_3 \rightarrow IBUTALOH + .63 CO + .37 HOCH_2OOH + .16 OH + .16 HO_2$ | 1.0E-17*0.43 | Rickard and Pascoe (2009), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|---|
| G45238 | TrGTerCN | MBO + NO ₃ → LNMBOABO2 | 4.6E-14*EXP(-400./TEMP) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45239 | TrGTerC | LMBOABO2 + HO ₂ → LMBOABOOH | KR02H02(5) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45240a | TrGTerCN | LMBOABO2 + NO → LMBOABNO3 | KR02N0*(.67*alpha_AN(7,2,0,0,0,temp,cair)+.33*alpha_AN(7,1,0,0,0,temp,cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45240b | TrGTerCN | LMBOABO2 + NO → HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + NO ₂ | KR02N0*(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), Taraborrelli (2016) |
| G45240c | TrGTerCN | LMBOABO2 + NO → IBUTALOH + HCHO + HO ₂ + NO ₂ | KR02N0*(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), Taraborrelli (2016) |
| G45241a | TrGTerC | LMBOABO2 → HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂ | k1_R02s0R02*.67 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45241b | TrGTerC | LMBOABO2 → IBUTALOH + HCHO + HO ₂ | k1_R02p0R02*.33 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45242a | TrGTerC | LMBOABOOH + OH → MBOACO | .67*2.93E-11+.33*2.05E-12 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45242b | TrGTerC | LMBOABOOH + OH → LMBOABO2 | .6*k_CH300H_OH | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45243 | TrGTerCN | LMBOABNO3 + OH → MBOACO + NO ₂ | .67*1.75E-12+.33*2.69E-12 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45244 | TrGTerC | MBOACO + OH → MBOCOCO + HO ₂ | 3.79E-12 | Rickard and Pascoe (2009) |
| G45245 | TrGTerC | MBOCOCO + OH → CO + IPRHOCO3 | 1.38E-11 | Rickard and Pascoe (2009) |
| G45246 | TrGTerCN | LNMBOABO2 + HO ₂ → LNMBOABOOH | KR02H02(5) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45247 | TrGTerCN | LNMBOABO2 + NO → .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009), Taraborrelli (2016)* |
| G45248 | TrGTerCN | LNMBOABO2 + NO ₃ → .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45249 | TrGTerCN | LNMBOABO2 → .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂ | k1_R02s0R02 | Rickard and Pascoe (2009), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|----------------------------|--|
| G45250a | TrGTerCN | LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBOCO | .65*4.89E-12+.35*2.52E-12 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45250b | TrGTerCN | LNMBOABOOH + OH → LNMBOABO2 | .6*k_CH300H_OH | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45251 | TrGTerCN | NMBOBOCO + OH → NC4OHCO3 | 4.26E-12 | Rickard and Pascoe (2009) |
| G45252a | TrGTerCN | NC4OHCO3 + HO ₂ → IBUTALOH + CO ₂ + NO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45252b | TrGTerCN | NC4OHCO3 + HO ₂ → NC4OHCO3H | KAPH02*(rco3_o3+rco3_ooh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| 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 | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G45256 | TrGTerCN | NC4OHCO3 → IBUTALOH + CO ₂ + NO ₂ | k1_R02RCO3 | 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 ₃ COCH ₃ + HCHO + CO ₂ + NO ₂ | 1.23E-12 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45400 | TrGAroCN | NC4MDCO2HN + OH → MMALANHY + NO ₂ | 0.6*k_CH300H_OH | Rickard and Pascoe (2009)* |
| G45401 | TrGAroCN | C54CO + NO ₃ → 3 CO + CH ₃ C(O)OO + HNO ₃ | KN03AL*5.5 | Rickard and Pascoe (2009) |
| G45402 | TrGAroC | C54CO + OH → 3 CO + CH ₃ C(O)OO | 1.72E-11 | Rickard and Pascoe (2009) |
| G45403a | TrGAroCN | NTLFUO2 + HO ₂ → NTLFUOOH | KR02H02(5)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G45403b | TrGAroCN | NTLFUO2 + HO ₂ → ACCOMECHO + NO ₂ + OH | KR02H02(5)*rcoch2o2_oh | Rickard and Pascoe (2009) |
| G45404 | TrGAroCN | NTLFUO2 + NO → ACCOMECHO + NO ₂ + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |
| G45405 | TrGAroCN | NTLFUO2 + NO ₃ → ACCOMECHO + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G45406 | TrGAroCN | NTLFUO2 → ACCOMECHO + NO ₂ | k1_R02t0R02 | 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 | KAPH02*(rco3_ooh+rco3_o3) | Rickard and Pascoe (2009) |
| G45411b | TrGAroC | C4CO2DBCO3 + HO ₂ → HO ₂ + CO + HCOCOCHO + CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45412 | TrGAroCN | C4CO2DBCO3 + NO → HO ₂ + CO + HCOCOCHO + CO ₂ + NO ₂ | KAPNO | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| G45413 | TrGAroCN | $C_4CO_2DBCO_3 + NO_2 \rightarrow C_4CO_2DBPAN$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G45414 | TrGAroCN | $C_4CO_2DBCO_3 + NO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G45415 | TrGAroC | $C_4CO_2DBCO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2$ | k1_R02RC03 | Rickard and Pascoe (2009) |
| G45416 | TrGAroC | $MMALANHY + OH \rightarrow MMALANHYO_2$ | 1.50E-12 | Rickard and Pascoe (2009) |
| G45421a | TrGAroC | $MMALANHYO_2 + HO_2 \rightarrow MMALNHYOOH$ | KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45421b | TrGAroC | $MMALANHYO_2 + HO_2 \rightarrow CO_2H_3CO_3 + CO_2 + OH$ | KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G45422 | TrGAroCN | $MMALANHYO_2 + NO \rightarrow CO_2H_3CO_3 + CO_2 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G45423 | TrGAroCN | $MMALANHYO_2 + NO_3 \rightarrow CO_2H_3CO_3 + CO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G45424 | TrGAroC | $MMALANHYO_2 \rightarrow CO_2H_3CO_3 + CO_2$ | k1_R02t0R02 | Rickard and Pascoe (2009)* |
| G45428 | TrGAroCN | $C_4CO_2DBPAN + OH \rightarrow HCOCOCHO + CO_2 + CO + NO_2$ | 2.74E-11 | Rickard and Pascoe (2009) |
| G45429 | TrGAroCN | $C_4CO_2DBPAN \rightarrow C_4CO_2DBCO_3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009)* |
| G45430a | TrGAroC | $C_5CO_14O_2 + HO_2 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH$ | KAPH02*rco3_oh | Rickard and Pascoe (2009)* |
| G45430b | TrGAroC | $C_5CO_14O_2 + HO_2 \rightarrow C_5CO_14OH + O_3$ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G45430c | TrGAroC | $C_5CO_14O_2 + HO_2 \rightarrow C_5CO_14OOH$ | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G45431 | TrGAroCN | $C_5CO_14O_2 + NO \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G45432 | TrGAroCN | $C_5CO_14O_2 + NO_2 \rightarrow C_5COO_2NO_2$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G45433 | TrGAroCN | $C_5CO_14O_2 + NO_3 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2$ | KR02N03*1.74 | Rickard and Pascoe (2009)* |
| G45434 | TrGAroC | $C_5CO_14O_2 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2$ | k1_R02RC03 | Rickard and Pascoe (2009)* |
| G45436 | TrGAroC | $C_5CO_14OH + OH \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2$ | 5.44E-11 | Rickard and Pascoe (2009)* |
| G45441 | TrGAroCN | $C_5DICARB + NO_3 \rightarrow C_5CO_14O_2 + HNO_3$ | KN03AL*2.75 | Rickard and Pascoe (2009) |
| G45442 | TrGAroC | $C_5DICARB + O_3 \rightarrow .5338 GLYOX + .063 CH_3CHO + .348 CH_3C(O)OO + .918 CO + .57 OH + .473 HO_2 + .0563 CH_3COCO_2H + .5338 MGLYOX + .676 H_2O_2 + .063 HCHO + .0563 HCOCO_2H + .2465 CO_2$ | 2.00E-18 | Rickard and Pascoe (2009) |
| G45443 | TrGAroC | $C_5DICARB + OH \rightarrow .48 C_5CO_14O_2 + .52 C_5DICARBO_2$ | 6.2E-11 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|----------------------------|
| 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 ₂ O ₂ | 8.00E-19 | see note* |
| G45453 | TrGAroC | TLFUONE + OH → TLFUO2 | 6.90E-11 | Rickard and Pascoe (2009) |
| G45454a | TrGAroC | ACCOMECO3 + HO ₂ → ACCOMECHO3 | KAPH02*(rco3_ooh+rco3_o3) | Rickard and Pascoe (2009) |
| G45454b | TrGAroC | ACCOMECO3 + HO ₂ → MECOACETO2 + CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G45455 | TrGAroCN | ACCOMECO3 + NO → MECOACETO2 + CO ₂ + NO ₂ | KAPNO | Rickard and Pascoe (2009) |
| G45456 | TrGAroCN | ACCOMECO3 + NO ₂ → ACCOMECHAN | k_CH3CO3_NO2 | Rickard and Pascoe (2009)* |
| G45457 | TrGAroCN | ACCOMECO3 + NO ₃ → MECOACETO2 + CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G45458 | TrGAroC | ACCOMECO3 → MECOACETO2 + CO ₂ | k1_R02RCO3 | Rickard and Pascoe (2009) |
| G45459 | TrGAroC | C4CO2DCO3H + OH → C4CO2DBC03 | 3.06E-11 | Rickard and Pascoe (2009) |
| G45464 | TrGAroCN | ACCOMECH0 + NO ₃ → ACCOMECHO3 + HNO ₃ | KN03AL*5.5 | Rickard and Pascoe (2009) |
| G45465 | TrGAroC | ACCOMECH0 + OH → ACCOMECHO3 | 7.09E-11 | Rickard and Pascoe (2009) |
| G45466 | TrGAroC | MMALNHOOH + 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 | 0.6*k_CH300H_OH | 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) |
| G45471 | TrGAroCN | ACCOMEPAN → ACCOMECHO3 + NO ₂ | k_PAN_M | Rickard and Pascoe (2009) |
| G45476a | TrGAroC | TLFUO2 + HO ₂ → TLFUOOH | KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G45476b | TrGAroC | TLFUO2 + HO ₂ → ACCOMECHO + HO ₂ + OH | KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh) | Rickard and Pascoe (2009)* |
| G45477 | TrGAroCN | TLFUO2 + NO → ACCOMECHO + HO ₂ + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |
| G45478 | TrGAroCN | TLFUO2 + NO ₃ → ACCOMECHO + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G45479 | TrGAroC | TLFUO2 → ACCOMECHO + HO ₂ | k1_R02t0R02 | 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 → ACCOMECHO3 | 3.59E-12 | Rickard and Pascoe (2009) |
| G45486a | TrGAroC | C5DIALO2 + HO ₂ → C5DIALOOH | KR02H02(5)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| G45486b | TrGAroC | $C5DIALO2 + HO_2 \rightarrow MALDIAL + CO + HO_2 + OH$ | $KR02H02(5)*rcoch2o2_oh$ | Rickard and Pascoe (2009)* |
| G45487 | TrGAroCN | $C5DIALO2 + NO \rightarrow MALDIAL + CO + HO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G45488 | TrGAroCN | $C5DIALO2 + NO_3 \rightarrow MALDIAL + CO + HO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G45489 | TrGAroC | $C5DIALO2 \rightarrow MALDIAL + CO + HO_2$ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G45490a | TrGAroC | $C5DICARBO2 + HO_2 \rightarrow C5DICAROOH$ | $KR02H02(5)*(rco3_ooh+rco3_o3)$ | Rickard and Pascoe (2009) |
| G45491b | TrGAroC | $C5DICARBO2 + HO_2 \rightarrow MGLYOX + GLYOX + HO_2 + OH$ | $KR02H02(5)*rco3_oh$ | Rickard and Pascoe (2009)* |
| G45492 | TrGAroCN | $C5DICARBO2 + NO \rightarrow MGLYOX + GLYOX + HO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G45493 | TrGAroCN | $C5DICARBO2 + NO_3 \rightarrow MGLYOX + GLYOX + HO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G45494 | TrGAroC | $C5DICARBO2 \rightarrow MGLYOX + GLYOX + HO_2$ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G46200a | TrGTerC | $CO235C6O2 + HO_2 \rightarrow CO235C6OOH$ | $KR02H02(6)*rcoch2o2_ooh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G46200b | TrGTerC | $CO235C6O2 + HO_2 \rightarrow CO23C4CO3 + HCHO + OH$ | $KR02H02(6)*rcoch2o2_oh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G46201 | TrGTerCN | $CO235C6O2 + NO \rightarrow CO23C4CO3 + HCHO + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46202 | TrGTerC | $CO235C6O2 \rightarrow CO23C4CO3 + HCHO$ | k1_R02p0R02 | Rickard and Pascoe (2009) |
| G46203 | TrGTerC | $CO235C6OOH + OH \rightarrow CO235C6O2$ | 1.01E-11 | Rickard and Pascoe (2009) |
| G46204 | TrGTerC | $C614O2 \rightarrow CO23C4CHO + HCHO + HO_2$ | k1_R02s0R02 | Rickard and Pascoe (2009) |
| G46205a | TrGTerCN | $C614O2 + NO \rightarrow CO23C4CHO + HCHO + HO_2 + NO_2$ | $KR02N0*(1.-alpha_AN(9,2,0,1,0,temp,cair))$ | Rickard and Pascoe (2009) |
| G46205b | TrGTerCN | $C614O2 + NO \rightarrow C614NO3$ | $KR02N0*alpha_AN(9,2,0,1,0,temp,cair)$ | Rickard and Pascoe (2009) |
| G46206a | TrGTerC | $C614O2 + HO_2 \rightarrow C614OOH$ | $KR02H02(6)*(1.-rchohch2o2_oh)$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G46206b | TrGTerC | $C614O2 + HO_2 \rightarrow CO23C4CHO + HCHO + HO_2 + OH$ | $KR02H02(6)*rchohch2o2_oh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| 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 | $CO235C5CHO + NO_3 \rightarrow CO23C4CO3 + CO + HNO_3$ | KN03AL*5.5 | Rickard and Pascoe (2009) |
| G46400 | TrGAroC | $PHENO2 + OH \rightarrow PHENO2$ | 1.16E-10 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|----------------------------|
| G46401 | TrGAroC | $C6CO4DB + OH \rightarrow CO + CO + HO_2 + CO + HCOCOCHO$ | 7.70E-11 | Rickard and Pascoe (2009) |
| G46402 | TrGAroC | $C5CO2DCO3H + OH \rightarrow C5CO2DBC03$ | 3.60E-11 | Rickard and Pascoe (2009) |
| G46403 | TrGAroCN | $NDNPHEOOH + OH \rightarrow NDNPHENO2$ | $0.6 * k_{CH300H_OH}$ | Rickard and Pascoe (2009) |
| G46404a | TrGAroC | $C615CO2O2 + HO_2 \rightarrow C615CO2OOH$ | $KR02H02(6) * (1 - r_{coch2o2_oh})$ | Rickard and Pascoe (2009) |
| G46404b | TrGAroC | $C615CO2O2 + HO_2 \rightarrow C5DICARB + CO + HO_2 + OH$ | $KR02H02(6) * r_{coch2o2_oh}$ | Rickard and Pascoe (2009)* |
| G46405 | TrGAroCN | $C615CO2O2 + NO \rightarrow C5DICARB + CO + HO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46406 | TrGAroCN | $C615CO2O2 + NO_3 \rightarrow C5DICARB + CO + HO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46407 | TrGAroC | $C615CO2O2 \rightarrow C5DICARB + CO + HO_2$ | $k1_R02s0R02$ | 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 | $NDNPHEO2 + HO_2 \rightarrow NDNPHENO0H$ | $KR02H02(6) * (1 - r_{chohch2o2_oh})$ | Rickard and Pascoe (2009) |
| G46413b | TrGAroCN | $NDNPHEO2 + HO_2 \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH$ | $KR02H02(6) * r_{chohch2o2_oh}$ | Rickard and Pascoe (2009)* |
| G46414 | TrGAroCN | $NDNPHEO2 + NO \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46415 | TrGAroCN | $NDNPHEO2 + NO_3 \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46416 | TrGAroCN | $NDNPHEO2 \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2$ | $k1_R02ISOPD02$ | Rickard and Pascoe (2009)* |
| G46417 | TrGAroC | $PBZQCO + OH \rightarrow C5CO2OHCO3$ | 6.07E-11 | Rickard and Pascoe (2009) |
| G46418 | TrGAroCN | $CATECHOL + NO_3 \rightarrow CATEC1O + HNO_3$ | 9.9E-11 | Rickard and Pascoe (2009)* |
| G46419 | TrGAroC | $CATECHOL + O_3 \rightarrow MALDALCO2H + HCOCO_2H + HO_2 + OH$ | 9.2E-18 | Rickard and Pascoe (2009) |
| G46420 | TrGAroC | $CATECHOL + OH \rightarrow CATEC1O$ | 1.0E-10 | Rickard and Pascoe (2009) |
| G46421 | TrGAroC | $C5COOHCO3H + OH \rightarrow C5CO2OHCO3$ | 8.01E-11 | Rickard and Pascoe (2009) |
| G46422 | TrGAroCN | $NCATECHOL + NO_3 \rightarrow NNCATECO2$ | 2.60E-12 | Rickard and Pascoe (2009) |
| G46423 | TrGAroCN | $NCATECHOL + OH \rightarrow NCATECO2$ | 3.47E-12 | Rickard and Pascoe (2009) |
| G46424a | TrGAroC | $C5CO2OHCO3 + HO_2 \rightarrow C5COOHCO3H$ | $KAPH02 * (r_{co3_ooh} + r_{co3_o3})$ | Rickard and Pascoe (2009) |
| G46424b | TrGAroC | $C5CO2OHCO3 + HO_2 \rightarrow HOCOC4DIAL + HO_2 + CO + CO_2 + OH$ | $KAPH02 * r_{co3_oh}$ | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|------------------------------|----------------------------|
| G46425 | TrGAroCN | $C_5CO_2OHCO_3 + NO \rightarrow HOCOC_4DIAL + HO_2 + CO + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G46426 | TrGAroCN | $C_5CO_2OHCO_3 + NO_2 \rightarrow C_5CO_2OHPAN$ | k_CH3C03_NO2 | Rickard and Pascoe (2009)* |
| G46427 | TrGAroCN | $C_5CO_2OHCO_3 + NO_3 \rightarrow HOCOC_4DIAL + HO_2 + CO + CO_2 + NO_2$ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G46428 | TrGAroC | $C_5CO_2OHCO_3 \rightarrow HOCOC_4DIAL + HO_2 + CO + CO_2$ | k1_R02RC03 | Rickard and Pascoe (2009) |
| G46429 | TrGAroCN | $BZEPOXMUC + NO_3 \rightarrow BZEMUCCO_3 + HNO_3$ | 2*KN03AL*2.75 | Rickard and Pascoe (2009) |
| G46430 | TrGAroC | $BZEPOXMUC + O_3 \rightarrow EPXC_4DIAL + .125 HCHO + .1125 HCOCO_2H + .0675 GLYOX + .0675 H_2O_2 + .82 HO_2 + .57 OH + 1.265 CO + .25 CO_2$ | 2.00E-18 | Rickard and Pascoe (2009)* |
| G46431 | TrGAroC | $BZEPOXMUC + OH \rightarrow .31 BZEMUCCO_3 + .69 BZEMUCO_2$ | 6.08E-11 | Rickard and Pascoe (2009) |
| G46432a | TrGAroCN | $NCATECO_2 + HO_2 \rightarrow NCATECOOH$ | KR02H02(6)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G46432b | TrGAroCN | $NCATECO_2 + HO_2 \rightarrow NC_4DCO_2H + HCOCO_2H + HO_2 + OH$ | KR02H02(6)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G46433 | TrGAroCN | $NCATECO_2 + NO \rightarrow NC_4DCO_2H + HCOCO_2H + HO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46434 | TrGAroCN | $NCATECO_2 + NO_3 \rightarrow NC_4DCO_2H + HCOCO_2H + HO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46435 | TrGAroCN | $NCATECO_2 \rightarrow NC_4DCO_2H + HCOCO_2H + HO_2$ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G46436 | TrGAroCN | $NPHEN1OOH + OH \rightarrow NPHEN1O_2$ | 9.00E-13 | Rickard and Pascoe (2009) |
| G46437a | TrGAroCN | $NPHENO_2 + HO_2 \rightarrow NPHENOOH$ | KR02H02(6)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G46437b | TrGAroCN | $NPHENO_2 + HO_2 \rightarrow MALDALCO_2H + GLYOX + NO_2 + OH$ | KR02H02(6)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G46438 | TrGAroCN | $NPHENO_2 + NO \rightarrow MALDALCO_2H + GLYOX + NO_2 + NO_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46439 | TrGAroCN | $NPHENO_2 + NO_3 \rightarrow MALDALCO_2H + GLYOX + NO_2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46440 | TrGAroCN | $NPHENO_2 \rightarrow MALDALCO_2H + GLYOX + NO_2$ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G46441 | TrGAroC | $BENZENE + OH \rightarrow .352 BZBIPERO_2 + .118 BZEPOXMUC + .118 HO_2 + .53 PHENOL + .53 HO_2$ | 2.3E-12*EXP(-190/TEMP) | Rickard and Pascoe (2009)* |
| G46442 | TrGAroCN | $C_5CO_2OHPAN + OH \rightarrow HOCOC_4DIAL + CO + CO + NO_2$ | 7.66E-11 | Rickard and Pascoe (2009) |
| G46443 | TrGAroCN | $C_5CO_2OHPAN \rightarrow C_5CO_2OHCO_3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|------------------------------|--|
| G46444 | TrGAroCN | CATEC1O + NO ₂ → NCATECHOL | k_C6H50_N02 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G46445 | TrGAroC | CATEC1O + O ₃ → CATEC1O2 | k_C6H50_03 | 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 | KR02H02(6)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G46447b | TrGAroCN | NNCATECO2 + HO ₂ → NC4DCO2H + HCOCO ₂ H + NO ₂ + OH | KR02H02(6)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G46448 | TrGAroCN | NNCATECO2 + NO → NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G46449 | TrGAroCN | NNCATECO2 + NO ₃ → NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G46450 | TrGAroCN | NNCATECO2 → NC4DCO2H + HCOCO ₂ H + NO ₂ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G46451 | TrGAroC | BZEMUCCO2H + OH → C5DIALO2 + CO ₂ | 4.06E-11 | Rickard and Pascoe (2009) |
| G46452 | TrGAroCN | NNCATECOOH + OH → NNCATECO2 | 0.6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G46453 | TrGAroCN | NPHEN1O + NO ₂ → DNPHEN | k_C6H50_N02 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G46454 | TrGAroCN | NPHEN1O + O ₃ → NPHEN1O2 | k_C6H50_03 | 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 → DNPHEO2 | 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 → PHENO2OH | KR02H02(6)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G46461b | TrGAroC | PHENO2 + HO ₂ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + OH | KR02H02(6)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G46462 | TrGAroCN | PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G46463 | TrGAroCN | PHENO2 + NO ₃ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|---|
| G46464 | TrGAroC | PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G46465 | TrGAroC | C615CO2OOH + OH → C6125CO + OH | 9.42E-11 | Rickard and Pascoe (2009) |
| G46466a | TrGAroC | C5CO2DBCO3 + HO ₂ → C5CO2DCO3H | KAPH02*(rco3_ooH+rco3_o3) | Rickard and Pascoe (2009) |
| G46466b | TrGAroC | C5CO2DBCO3 + HO ₂ → CH ₃ C(O) + HCOCOCHO + CO ₂ + OH | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G46467 | TrGAroCN | C5CO2DBCO3 + NO → CH ₃ C(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 ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G46470 | TrGAroC | C5CO2DBCO3 → CH ₃ C(O) + HCOCOCHO + CO ₂ | k1_R02RCO3 | Rickard and Pascoe (2009) |
| G46471 | TrGAroCN | NPHEN1O2 + HO ₂ → NPHEN1OOH | KR02H02(6) | Rickard and Pascoe (2009) |
| G46472a | TrGAroCN | NPHEN1O2 + NO → NPHEN1O + NO ₂ | KR02N0 | 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 | KR02N03 | Rickard and Pascoe (2009) |
| G46474 | TrGAroCN | NPHEN1O2 → NPHEN1O | k1_R02sR02 | Rickard and Pascoe (2009) |
| 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 | 0.6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G46479 | TrGAroC | PBZQOOH + OH → PBZQCO + OH | 1.23E-10 | Rickard and Pascoe (2009) |
| G46480a | TrGAroC | PBZQO2 + HO ₂ → PBZQOOH | KR02H02(6)*(1-rchohch2o2_oh-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G46480b | TrGAroC | PBZQO2 + HO ₂ → C5CO2OHCO3 + OH | KR02H02(6)*(rchohch2o2_oh+rcoch2o2_oh) | Rickard and Pascoe (2009)* |
| G46481 | TrGAroCN | PBZQO2 + NO → C5CO2OHCO3 + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G46482 | TrGAroCN | PBZQO2 + NO ₃ → C5CO2OHCO3 + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G46483 | TrGAroC | PBZQO2 → C5CO2OHCO3 | k1_R02sOR02 | Rickard and Pascoe (2009)* |
| G46484 | TrGAroC | BZOBIPEROH + OH → MALDIALCO3 + GLYOX | 8.16E-11 | Rickard and Pascoe (2009) |
| G46485a | TrGAroCN | DNPHENO2 + HO ₂ → DNPHENOOH | KR02H02(6)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G46485b | TrGAroCN | DNPHENO2 + HO ₂ → NC4DCO2H + HCOCO ₂ H + NO ₂ + OH | KR02H02(6)*rchohch2o2_oh | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|----------------------------|
| G46486 | TrGAroCN | $\text{DNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2 + \text{NO}_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46487 | TrGAroCN | $\text{DNPHENO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2 + \text{NO}_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46488 | TrGAroCN | $\text{DNPHENO2} \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2$ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G46489 | TrGAroC | $\text{BZBIPEROOH} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{OH}$ | 9.77E-11 | Rickard and Pascoe (2009) |
| G46490a | TrGAroC | $\text{BZEMUCO2} + \text{HO}_2 \rightarrow \text{BZEMUCOOH}$ | KR02H02(6) | Rickard and Pascoe (2009) |
| G46490b | TrGAroC | $\text{BZEMUCO2} + \text{HO}_2 \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{OH}$ | KR02H02(6) | Rickard and Pascoe (2009)* |
| G46491a | TrGAroCN | $\text{BZEMUCO2} + \text{NO} \rightarrow \text{BZEMUCNO3}$ | KR02N0*alpha_AN(10,2,0,1,0, temp, cair) | Rickard and Pascoe (2009) |
| G46491b | TrGAroCN | $\text{BZEMUCO2} + \text{NO} \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{NO}_2$ | KR02N0*(1.-alpha_AN(10,2,0,1,0, temp, cair)) | Rickard and Pascoe (2009)* |
| G46492 | TrGAroCN | $\text{BZEMUCO2} + \text{NO}_3 \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{NO}_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46493 | TrGAroC | $\text{BZEMUCO2} \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO}$ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G46494 | TrGAroCN | $\text{C5CO2DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2$ | 3.28E-11 | Rickard and Pascoe (2009) |
| G46495 | TrGAroCN | $\text{C5CO2DBPAN} \rightarrow \text{C5CO2DBCO3} + \text{NO}_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G46496 | TrGAroCN | $\text{NBZQOOH} + \text{OH} \rightarrow \text{NBZQO2}$ | 6.68E-11 | Rickard and Pascoe (2009) |
| G46497 | TrGAroC | $\text{CATEC1OOH} + \text{OH} \rightarrow \text{CATEC1O2}$ | .6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G46498 | TrGAroC | $\text{C6125CO} + \text{OH} \rightarrow \text{C5CO14O2} + \text{CO}$ | 6.45E-11 | Rickard and Pascoe (2009) |
| G46499a | TrGAroCN | $\text{NBZQO2} + \text{HO}_2 \rightarrow \text{NBZQOOH}$ | KR02H02(6)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G46499b | TrGAroCN | $\text{NBZQO2} + \text{HO}_2 \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$ | KR02H02(6)*rcoch2o2_oh | Rickard and Pascoe (2009)* |
| G46500 | TrGAroCN | $\text{NBZQO2} + \text{NO} \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{NO}_2$ | KR02N0 | Rickard and Pascoe (2009)* |
| G46501 | TrGAroCN | $\text{NBZQO2} + \text{NO}_3 \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{NO}_2$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46502 | TrGAroCN | $\text{NBZQO2} \rightarrow \text{C6CO4DB} + \text{NO}_2$ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G46503 | TrGAroCN | $\text{DNPHENO2} + \text{OH} \rightarrow \text{DNPHENO2}$ | 0.6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G46504 | TrGAroC | $\text{CATEC1O2} + \text{HO}_2 \rightarrow \text{CATEC1OOH}$ | KR02H02(6) | Rickard and Pascoe (2009) |
| G46505a | TrGAroCN | $\text{CATEC1O2} + \text{NO} \rightarrow \text{CATEC1O} + \text{NO}_2$ | KR02N0 | Rickard and Pascoe (2009) |
| G46505b | TrGAroCN | $\text{CATEC1O2} + \text{NO}_2 \rightarrow \text{CATEC1O} + \text{NO}_3$ | K_C6H502_N02 | Jagiella and Zabel (2007)* |
| G46506 | TrGAroCN | $\text{CATEC1O2} + \text{NO}_3 \rightarrow \text{CATEC1O} + \text{NO}_2$ | KR02N03 | Rickard and Pascoe (2009) |
| G46507 | TrGAroC | $\text{CATEC1O2} \rightarrow \text{CATEC1O}$ | k1_R02s0R02 | Rickard and Pascoe (2009) |
| G46508 | TrGAroC | $\text{BZEMUCCO3H} + \text{OH} \rightarrow \text{BZEMUCCO3}$ | 4.37E-11 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|---|
| G46509 | TrGAroC | $C_6H_5OOH + OH \rightarrow C_6H_5O_2$ | 3.60E-12 | Rickard and Pascoe (2009) |
| G46510 | TrGAroC | $BZEMUCOOH + OH \rightarrow BZEMUCCO + OH$ | 1.31E-10 | Rickard and Pascoe (2009) |
| G46511a | TrGAroC | $BZEMUCCO_3 + HO_2 \rightarrow BZEMUCCO_2H + O_3$ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G46511b | TrGAroC | $BZEMUCCO_3 + HO_2 \rightarrow BZEMUCCO_3H$ | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G46511c | TrGAroC | $BZEMUCCO_3 + HO_2 \rightarrow C_5DIALO_2 + CO_2 + OH$ | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G46512 | TrGAroCN | $BZEMUCCO_3 + NO \rightarrow C_5DIALO_2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G46513 | TrGAroCN | $BZEMUCCO_3 + NO_2 \rightarrow BZEMUCPAN$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G46514 | TrGAroCN | $BZEMUCCO_3 + NO_3 \rightarrow C_5DIALO_2 + CO_2 + NO_2$ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G46515 | TrGAroC | $BZEMUCCO_3 \rightarrow C_5DIALO_2 + CO_2$ | k1_R02RCO3 | Rickard and Pascoe (2009)* |
| G46516 | TrGAroC | $C_6H_5O_2 + HO_2 \rightarrow C_6H_5OOH$ | KR02H02(6) | Rickard and Pascoe (2009) |
| G46517a | TrGAroCN | $C_6H_5O_2 + NO \rightarrow C_6H_5O + NO_2$ | KR02NO | Rickard and Pascoe (2009) |
| G46517b | TrGAroCN | $C_6H_5O_2 + NO_2 \rightarrow C_6H_5O + NO_3$ | K_C6H5O2_NO2 | Jagiella and Zabel (2007)* |
| G46518 | TrGAroCN | $C_6H_5O_2 + NO_3 \rightarrow C_6H_5O + NO_2$ | KR02N03 | Rickard and Pascoe (2009) |
| G46519 | TrGAroC | $C_6H_5O_2 \rightarrow C_6H_5O$ | k1_R02sR02 | Rickard and Pascoe (2009) |
| G46521 | TrGAroCN | $BZEMUCNO_3 + OH \rightarrow BZEMUCCO + NO_2$ | 4.38E-11 | Rickard and Pascoe (2009) |
| G46522a | TrGAroC | $BZBIPERO_2 + HO_2 \rightarrow BZBIPEROOH$ | KR02H02(6)*(1.-rbipero2_oh) | Rickard and Pascoe (2009) |
| G46522b | TrGAroC | $BZBIPERO_2 + HO_2 \rightarrow OH + GLYOX + HO_2 + .5$ $BZFUONE + .5 BZFUONE$ | KR02H02(6)*rbipero2_oh | Rickard and Pascoe (2009), Bird- sall et al. (2010)* |
| G46523a | TrGAroCN | $BZBIPERO_2 + NO \rightarrow BZBIPERNO_3$ | KR02N0*alpha_AN(9,2,0,0,1,temp, cair) | Rickard and Pascoe (2009) |
| G46523b | TrGAroCN | $BZBIPERO_2 + NO \rightarrow NO_2 + GLYOX + HO_2 + .5$ $BZFUONE + .5 BZFUONE$ | KR02N0*(1.-alpha_AN(9,2,0,0,1, temp,cair)) | Rickard and Pascoe (2009)* |
| G46524 | TrGAroCN | $BZBIPERO_2 + NO_3 \rightarrow NO_2 + GLYOX + HO_2 + .5$ $BZFUONE + .5 BZFUONE$ | KR02N03 | Rickard and Pascoe (2009)* |
| G46525 | TrGAroC | $BZBIPERO_2 \rightarrow GLYOX + HO_2 + BZFUONE$ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G47200 | TrGTerCN | $CO_235C_6CHO + NO_3 \rightarrow CO_235C_6CO_3 + HNO_3$ | KN03AL*5.5 | Rickard and Pascoe (2009) |
| G47201 | TrGTerC | $CO_235C_6CHO + OH \rightarrow CO_235C_6CO_3$ | 6.70E-11 | Rickard and Pascoe (2009) |
| G47202a | TrGTerC | $CO_235C_6CO_3 + HO_2 \rightarrow C_235C_6CO_3H$ | KAPH02*(rco3_ooh+rco3_o3) | Rickard and Pascoe (2009) |
| G47202b | TrGTerC | $CO_235C_6CO_3 + HO_2 \rightarrow CO_235C_6O_2 + CO_2 + OH$ | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G47203 | TrGTerCN | $CO_235C_6CO_3 + NO \rightarrow CO_235C_6O_2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47204 | TrGTerCN | $CO_235C_6CO_3 + NO_2 \rightarrow C_7PAN_3$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G47205 | TrGTerC | $CO_235C_6CO_3 \rightarrow CO_235C_6O_2 + CO_2$ | k1_R02RCO3 | Rickard and Pascoe (2009) |
| G47206 | TrGTerC | $C_235C_6CO_3H + OH \rightarrow CO_235C_6CO_3$ | 4.75E-12 | Rickard and Pascoe (2009) |
| G47207 | TrGTerCN | $C_7PAN_3 + OH \rightarrow CO_235C_5CHO + CO + NO_2$ | 8.83E-13 | Rickard and Pascoe (2009) |
| G47208 | TrGTerCN | $C_7PAN_3 \rightarrow CO_235C_6CO_3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|---|--|
| G47209a | TrGTerC | $C716O2 + HO_2 \rightarrow C716OOH$ | $KR02H02(7)*rcoch2o2_ooh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G47209b | TrGTerC | $C716O2 + HO_2 \rightarrow CO13C4CHO + CH_3C(O) + OH$ | $KR02H02(7)*rcoch2o2_oh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G47210 | TrGTerCN | $C716O2 + NO \rightarrow CO13C4CHO + CH_3C(O) + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G47211 | TrGTerC | $C716O2 \rightarrow CO13C4CHO + CH_3C(O)$ | k1_R02s0R02 | Rickard and Pascoe (2009) |
| G47212 | TrGTerC | $C716OOH + OH \rightarrow CO235C6CHO + OH$ | 1.20E-10 | Rickard and Pascoe (2009) |
| G47213 | TrGTerC | $C721O2 + HO_2 \rightarrow C721OOH$ | KR02H02(7) | Rickard and Pascoe (2009) |
| G47214 | TrGTerCN | $C721O2 + NO \rightarrow C722O2 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G47215 | TrGTerC | $C721O2 \rightarrow C722O2$ | k1_R02pR02 | Rickard and Pascoe (2009) |
| G47216 | TrGTerC | $C721OOH + OH \rightarrow C721O2$ | 1.27E-11 | Rickard and Pascoe (2009) |
| G47217 | TrGTerC | $C722O2 + HO_2 \rightarrow C722OOH$ | KR02H02(7) | Rickard and Pascoe (2009) |
| G47218 | TrGTerCN | $C722O2 + NO \rightarrow CH_3COCH_3 + C44O2 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G47219 | TrGTerC | $C722O2 \rightarrow CH_3COCH_3 + C44O2$ | k1_R02tR02 | Rickard and Pascoe (2009) |
| G47220 | TrGTerC | $C722OOH + OH \rightarrow C722O2$ | 3.31E-11 | Rickard and Pascoe (2009) |
| G47221 | TrGTerC | $ROO6R3O2 \rightarrow ROO6R5O2$ | $5.68E10*EXP(-8745./TEMP)$ | Vereecken and Peeters (2012) |
| G47222 | TrGTerCN | $ROO6R3O2 + NO \rightarrow ROO6R3O + NO_2$ | KR02NO | Vereecken and Peeters (2012)* |
| G47223 | TrGTerC | $ROO6R3O2 + HO_2 \rightarrow 7\text{ L CARBON}$ | KR02H02(7) | Vereecken and Peeters (2012)* |
| G47224 | TrGTerC | $ROO6R3O2 \rightarrow ROO6R3O$ | k1_R02sR02 | Vereecken and Peeters (2012) |
| G47225 | TrGTerC | $ROO6R3O \rightarrow 7\text{ L CARBON} + HO_2$ | $5.7E10*EXP(-2949./TEMP)$ | Vereecken and Peeters (2012)* |
| G47226 | TrGTerC | $ROO6R5O2 \rightarrow 7\text{ L CARBON} + OH$ | $9.17E10*EXP(-8706./TEMP)$ | Vereecken and Peeters (2012)* |
| G47400 | TrGAroC | $TOLUENE + OH \rightarrow .07\text{ C6H5CH2O2} + .18\text{ CRESOL} + .18\text{ HO}_2 + .65\text{ TLBIPERO2} + .10\text{ TLEPOXMUC} + .10\text{ HO}_2$ | $1.8E-12*EXP(340/TEMP)$ | Rickard and Pascoe (2009)* |
| G47401 | TrGAroC | $C6H5CH2O2 + HO_2 \rightarrow C6H5CH2OOH$ | $1.5E-13*EXP(1310/TEMP)$ | Rickard and Pascoe (2009) |
| G47402a | TrGAroCN | $C6H5CH2O2 + NO \rightarrow C6H5CH2NO3$ | $KR02NO*\alpha_AN(7,1,0,0,0,temp, cair)$ | Rickard and Pascoe (2009)* |
| G47402b | TrGAroCN | $C6H5CH2O2 + NO \rightarrow BENZAL + HO_2 + NO_2$ | $KR02NO*(1.-\alpha_AN(7,1,0,0,0,temp, cair))$ | Rickard and Pascoe (2009)* |
| G47403 | TrGAroCN | $C6H5CH2O2 + NO_3 \rightarrow BENZAL + HO_2 + NO_2$ | KR02NO3 | Rickard and Pascoe (2009)* |
| G47404 | TrGAroC | $C6H5CH2O2 \rightarrow BENZAL + HO_2$ | $2*(k_CH302*2.4E-14*EXP(1620./TEMP))**0.5*R02$ | Rickard and Pascoe (2009)* |
| G47405 | TrGAroCN | $CRESOL + NO_3 \rightarrow .103\text{ CRESO2} + .103\text{ HNO}_3 + .506\text{ NCRESO2} + .391\text{ TOL1O} + .391\text{ HNO}_3$ | 1.4E-11 | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|---|
| 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 | KR02H02(7)*(1.-rbipero2_oh) | Rickard and Pascoe (2009) |
| G47407b | TrGAroC | TLBIPERO2 + HO ₂ → OH + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | KR02H02(7)*rbipero2_oh | Rickard and Pascoe (2009), Bird-sall et al. (2010)* |
| G47408a | TrGAroCN | TLBIPERO2 + NO → NO ₂ + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | KR02N0*(1.-alpha_AN(11,2,0,0,1,temp,cair)) | Rickard and Pascoe (2009)* |
| G47408b | TrGAroCN | TLBIPERO2 + NO → TLBIPERNO3 | KR02N0*alpha_AN(11,2,0,0,1,temp,cair) | Rickard and Pascoe (2009)* |
| G47409 | TrGAroCN | TLBIPERO2 + NO ₃ → NO ₂ + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | KR02N03 | Rickard and Pascoe (2009)* |
| G47410 | TrGAroC | TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G47411 | TrGAroCN | TLEPOXMUC + NO ₃ → TLEMUCCO3 + HNO ₃ | KN03AL*2.75 | Rickard and Pascoe (2009) |
| G47412 | TrGAroC | TLEPOXMUC + O ₃ → EPXC4DIAL + .125 CH ₃ CHO + .695 CH ₃ C(O) + .57 CO + .57 OH + .125 HO ₂ + .1125 CH ₃ COCO ₂ H + .0675 MGLYOX + .0675 H ₂ O 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 | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G47418b | TrGAroC | CRESO2 + HO ₂ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47419 | TrGAroCN | CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47420 | TrGAroCN | CRESO2 + NO ₃ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|---|
| G47421 | TrGAroC | CRESO2 → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G47422a | TrGAroCN | NCRESO2 + HO ₂ → NCRESOOH | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G47422b | TrGAroCN | NCRESO2 + HO ₂ → C5CO14OH + GLYOX + NO ₂ + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47423 | TrGAroCN | NCRESO2 + NO → C5CO14OH + GLYOX + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47424 | TrGAroCN | NCRESO2 + NO ₃ → C5CO14OH + GLYOX + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47425 | TrGAroCN | NCRESO2 → C5CO14OH + GLYOX + NO ₂ | k1_R02ISOPD02 | Rickard and Pascoe (2009)* |
| G47426 | TrGAroCN | TOL1O + NO ₂ → TOL1OHNO2 | k_C6H50_N02 | Rickard and Pascoe (2009), Platz et al. (1998)* |
| G47427 | TrGAroC | TOL1O + O ₃ → OXYL1O2 | k_C6H50_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 ₂ H + 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 | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G47434b | TrGAroC | TLEMUCCO3 + HO ₂ → TLEMUCCO2H + O ₃ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G47434c | TrGAroC | TLEMUCCO3 + HO ₂ → TLEMUCCO3H | KAPH02*rco3_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_CH3C03_N02 | Rickard and Pascoe (2009)* |
| G47437 | TrGAroCN | TLEMUCCO3 + NO ₃ → C615CO2O2 + CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G47438 | TrGAroC | TLEMUCCO3 → C615CO2O2 + CO ₂ | k1_R02RC03 | Rickard and Pascoe (2009)* |
| G47439a | TrGAroC | TLEMUCO2 + HO ₂ → TLEMUCOOH | KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G47439b | TrGAroC | TLEMUCO2 + HO ₂ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH | KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh) | Rickard and Pascoe (2009)* |
| G47440a | TrGAroCN | TLEMUCO2 + NO → TLEMUCNO3 | KR02N0*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 | KR02N0*(1.-alpha_AN(11,2,1,0,0,temp,cair)) | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|-----------------------------|--|
| G47441 | TrGAroCN | TLEMUCO2 + NO ₃ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47442 | TrGAroC | TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ | k1_R02s0R02 | 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)* |
| G47446 | TrGAroCN | C6H5CO3 + NO ₃ → C6H5O2 + CO ₂ + NO ₂ | KR02N03*1.74 | Rickard and Pascoe (2009) |
| G47447 | TrGAroC | C6H5CO3 → C6H5O2 + CO ₂ | k1_R02RC03 | 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 | KR02H02(7) | Rickard and Pascoe (2009) |
| G47453 | TrGAroCN | OXYL1O2 + NO → TOL1O + NO ₂ | KR02N0 | 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 | KR02N03 | Rickard and Pascoe (2009) |
| G47456 | TrGAroC | OXYL1O2 → TOL1O | k1_R02sR02 | Rickard and Pascoe (2009) |
| G47457 | TrGAroCN | MCATEC1O + NO ₂ → MNCATECH | k_C6H50_NO2 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G47458 | TrGAroC | MCATEC1O + O ₃ → MCATEC1O2 | k_C6H50_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 ₃ C(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) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|--|
| 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_C6H50_N02 | Rickard and Pascoe (2009), Platz et al. (1998) |
| G47473 | TrGAroCN | NCRES1O + O ₃ → NCRES1O2 | k_C6H50_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) |
| G47477 | TrGAroC | MCATEC1O2 + HO ₂ → MCATEC1OOH | KR02H02(7) | Rickard and Pascoe (2009) |
| G47478 | TrGAroCN | MCATEC1O2 + NO → MCATEC1O + NO ₂ | KR02N0 | Rickard and Pascoe (2009) |
| G47479 | TrGAroCN | MCATEC1O2 + NO ₂ → MCATEC1O + NO ₃ | K_C6H502_N02 | Jagiella and Zabel (2007)* |
| G47480 | TrGAroCN | MCATEC1O2 + NO ₃ → MCATEC1O + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G47481 | TrGAroC | MCATEC1O2 → MCATEC1O | k1_R02s0R02 | Rickard and Pascoe (2009) |
| G47482a | TrGAroCN | NPTLQO2 + HO ₂ → NPTLQOOH | KR02H02(7)*(1-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G47482b | TrGAroCN | NPTLQO2 + HO ₂ → C7CO4DB + NO ₂ + OH | KR02H02(7)*rcoch2o2_oh | Rickard and Pascoe (2009)* |
| G47483 | TrGAroCN | NPTLQO2 + NO → C7CO4DB + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47484 | TrGAroCN | NPTLQO2 + NO ₃ → C7CO4DB + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47485 | TrGAroCN | NPTLQO2 → C7CO4DB + NO ₂ | k1_R02s0R02 | Rickard and Pascoe (2009)* |
| G47486a | TrGAroC | PTLQO2 + HO ₂ → PTLQOOH | KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh) | Rickard and Pascoe (2009) |
| G47486b | TrGAroC | PTLQO2 + HO ₂ → C6CO2OHCO3 + OH | KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh) | Rickard and Pascoe (2009)* |
| G47487 | TrGAroCN | PTLQO2 + NO → C6CO2OHCO3 + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47488 | TrGAroCN | PTLQO2 + NO ₃ → C6CO2OHCO3 + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47489 | TrGAroC | PTLQO2 → C6CO2OHCO3 | k1_R02s0R02 | 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 | KR02H02(7) | Rickard and Pascoe (2009) |
| G47493 | TrGAroCN | NCRES1O2 + NO → NCRES1O + NO ₂ | KR02N0 | Rickard and Pascoe (2009) |
| G47494 | TrGAroCN | NCRES1O2 + NO ₂ → NCRES1O + NO ₃ | K_C6H502_N02 | Jagiella and Zabel (2007)* |
| G47495 | TrGAroCN | NCRES1O2 + NO ₃ → NCRES1O + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G47496 | TrGAroCN | NCRES1O2 → NCRES1O | k1_R02sR02 | Rickard and Pascoe (2009) |
| G47497a | TrGAroCN | MNNCATECO2 + HO ₂ → MNNCATCOOH | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|------------------------------|----------------------------|
| G47497b | TrGAroCN | MNNCATECO ₂ + HO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47498 | TrGAroCN | MNNCATECO ₂ + NO → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47499 | TrGAroCN | MNNCATECO ₂ + NO ₃ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47500 | TrGAroCN | MNNCATECO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ | k1_R02IS0PD02 | Rickard and Pascoe (2009) |
| G47501a | TrGAroCN | MNCATECO ₂ + HO ₂ → MNCATECOOH | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G47501b | TrGAroCN | MNCATECO ₂ + HO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + HO ₂ + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47502 | TrGAroCN | MNCATECO ₂ + NO → NC ₄ MDCO ₂ HN + HCOCO ₂ H + HO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47503 | TrGAroCN | MNCATECO ₂ + NO ₃ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + HO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47504 | TrGAroCN | MNCATECO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + HO ₂ | k1_R02IS0PD02 | 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 → C6CO2OHC03 | 7.95E-11 | Rickard and Pascoe (2009) |
| G47509a | TrGAroCN | NDNCRESO ₂ + HO ₂ → NDNCRESOOH | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G47509b | TrGAroCN | NDNCRESO ₂ + HO ₂ → NC ₄ MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47510 | TrGAroCN | NDNCRESO ₂ + NO → NC ₄ MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47511 | TrGAroCN | NDNCRESO ₂ + NO ₃ → NC ₄ MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47512 | TrGAroCN | NDNCRESO ₂ → NC ₄ MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ | k1_R02IS0PD02 | Rickard and Pascoe (2009)* |
| G47513a | TrGAroCN | DNCRESO ₂ + HO ₂ → DNCRESOOH | KR02H02(7)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G47513b | TrGAroCN | DNCRESO ₂ + HO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + OH | KR02H02(7)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G47514 | TrGAroCN | DNCRESO ₂ + NO → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G47515 | TrGAroCN | DNCRESO ₂ + NO ₃ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009)* |
| G47516 | TrGAroCN | DNCRESO ₂ → NC ₄ MDCO ₂ HN + HCOCO ₂ H + NO ₂ | k1_R02IS0PD02 | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|----------------------------|
| G47517 | TrGAroCN | $\text{NCRES1OOH} + \text{OH} \rightarrow \text{NCRES1O2}$ | 1.53E-12 | Rickard and Pascoe (2009) |
| G47518 | TrGAroCN | $\text{MNNCATCOOH} + \text{OH} \rightarrow \text{MNNCATECO2}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009) |
| G47519 | TrGAroCN | $\text{MNCATECOOH} + \text{OH} \rightarrow \text{MNCATECO2}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009) |
| G47520 | TrGAroC | $\text{C7CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CH}_3\text{C(O)} + \text{HCOCOCHO}$ | 9.58E-11 | Rickard and Pascoe (2009) |
| G47521a | TrGAroC | $\text{C6CO2OHCO3} + \text{HO}_2 \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$ | $\text{KAPH02} \cdot \text{rco3_oh}$ | Rickard and Pascoe (2009) |
| G47521b | TrGAroC | $\text{C6CO2OHCO3} + \text{HO}_2 \rightarrow \text{C6COOHCO3H}$ | $\text{KAPH02} \cdot (\text{rco3_ooh} + \text{rco3_o3})$ | Rickard and Pascoe (2009) |
| G47522 | TrGAroCN | $\text{C6CO2OHCO3} + \text{NO} \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$ | KAPNO | Rickard and Pascoe (2009) |
| G47523 | TrGAroCN | $\text{C6CO2OHCO3} + \text{NO}_2 \rightarrow \text{C6CO2OHPAN}$ | $k_{\text{CH3C03_N02}}$ | Rickard and Pascoe (2009) |
| G47524 | TrGAroCN | $\text{C6CO2OHCO3} + \text{NO}_3 \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$ | $\text{KR02N03} \cdot 1.74$ | Rickard and Pascoe (2009) |
| G47525 | TrGAroC | $\text{C6CO2OHCO3} \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2$ | $k1_{\text{R02R03}}$ | Rickard and Pascoe (2009) |
| G47526 | TrGAroCN | $\text{NDNCRESOOH} + \text{OH} \rightarrow \text{NDNCRESO2}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009) |
| G47527 | TrGAroCN | $\text{DNCRESOOH} + \text{OH} \rightarrow \text{DNCRESO2}$ | $0.6 \cdot k_{\text{CH300H_OH}}$ | Rickard and Pascoe (2009) |
| G47528 | TrGAroC | $\text{C6COOHCO3H} + \text{OH} \rightarrow \text{C6CO2OHCO3}$ | 9.29E-11 | Rickard and Pascoe (2009) |
| G47529 | TrGAroCN | $\text{C6CO2OHPAN} + \text{OH} \rightarrow \text{C5134CO2OH} + \text{CO} + \text{CO} + \text{NO}_2$ | 8.96E-11 | Rickard and Pascoe (2009) |
| G47530 | TrGAroCN | $\text{C6CO2OHPAN} \rightarrow \text{C6CO2OHCO3} + \text{NO}_2$ | $k_{\text{PAN_M}}$ | Rickard and Pascoe (2009) |
| G48200 | TrGTerC | $\text{C85O2} \rightarrow \text{C86O2}$ | $k1_{\text{R02tR02}}$ | Rickard and Pascoe (2009) |
| G48201 | TrGTerC | $\text{C85O2} + \text{HO}_2 \rightarrow \text{C85OOH}$ | $\text{KR02H02} (8)$ | Rickard and Pascoe (2009) |
| G48202 | TrGTerCN | $\text{C85O2} + \text{NO} \rightarrow \text{C86O2} + \text{NO}_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G48203 | TrGTerC | $\text{C85OOH} + \text{OH} \rightarrow \text{C85O2}$ | 1.29E-11 | Rickard and Pascoe (2009) |
| G48204 | TrGTerC | $\text{C86O2} \rightarrow \text{C511O2} + \text{CH}_3\text{COCH}_3$ | $k1_{\text{R02tR02}}$ | Rickard and Pascoe (2009) |
| G48205 | TrGTerCN | $\text{C86O2} + \text{NO} \rightarrow \text{C511O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G48206 | TrGTerC | $\text{C86O2} + \text{HO}_2 \rightarrow \text{C86OOH}$ | $\text{KR02H02} (8)$ | Rickard and Pascoe (2009) |
| G48207 | TrGTerC | $\text{C86OOH} + \text{OH} \rightarrow \text{C86O2}$ | 3.45E-11 | Rickard and Pascoe (2009) |
| G48208 | TrGTerC | $\text{C811O2} \rightarrow \text{C812O2}$ | $k1_{\text{R02pR02}}$ | Rickard and Pascoe (2009) |
| G48209 | TrGTerC | $\text{C811O2} + \text{HO}_2 \rightarrow 8 \text{ L CARBON}$ | $\text{KR02H02} (8)$ | Rickard and Pascoe (2009) |
| G48210 | TrGTerCN | $\text{C811O2} + \text{NO} \rightarrow \text{C812O2} + \text{NO}_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G48211 | TrGTerC | $\text{C812O2} \rightarrow \text{C813O2}$ | $k1_{\text{R02t0R02}}$ | Rickard and Pascoe (2009) |
| G48212 | TrGTerCN | $\text{C812O2} + \text{NO} \rightarrow \text{C813O2} + \text{NO}_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G48213 | TrGTerC | $\text{C812O2} + \text{HO}_2 \rightarrow \text{C812OOH}$ | $\text{KR02H02} (8)$ | Rickard and Pascoe (2009) |
| G48214 | TrGTerC | $\text{C812OOH} + \text{OH} \rightarrow \text{C812O2}$ | 1.09E-11 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|----------------------------|
| G48215 | TrGTerC | $C813O2 \rightarrow CH_3COCH_3 + C512O2$ | k1_R02tR02 | Rickard and Pascoe (2009) |
| G48216 | TrGTerCN | $C813O2 + NO \rightarrow CH_3COCH_3 + C512O2 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G48217 | TrGTerC | $C813O2 + HO_2 \rightarrow C813OOH$ | KR02HO2(8) | Rickard and Pascoe (2009) |
| G48218 | TrGTerC | $C813OOH + OH \rightarrow C813O2$ | 1.86E-11 | Rickard and Pascoe (2009) |
| G48219 | TrGTerCN | $C721CHO + NO_3 \rightarrow C721CO3 + HNO_3$ | KN03AL*8.5 | Rickard and Pascoe (2009) |
| G48220 | TrGTerC | $C721CHO + OH \rightarrow C721CO3$ | 2.63E-11 | Rickard and Pascoe (2009) |
| G48221a | TrGTerC | $C721CO3 + HO_2 \rightarrow C721CO3H$ | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G48221b | TrGTerC | $C721CO3 + HO_2 \rightarrow C721O2 + CO_2 + OH$ | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G48221c | TrGTerC | $C721CO3 + HO_2 \rightarrow NORPINIC + O_3$ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G48222 | TrGTerCN | $C721CO3 + NO \rightarrow C721O2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009)* |
| G48223 | TrGTerCN | $C721CO3 + NO_2 \rightarrow C721PAN$ | k_CH3CO3_NO2 | Rickard and Pascoe (2009) |
| G48224 | TrGTerCN | $C721CO3 + NO_3 \rightarrow C721O2 + CO_2 + NO_2$ | KR02NO3*1.74 | Rickard and Pascoe (2009) |
| G48225 | TrGTerC | $C721CO3 \rightarrow C721O2 + CO_2$ | k1_R02RCO3*0.9 | Taraborrelli (2016) |
| G48226 | TrGTerC | $C721CO3 \rightarrow NORPINIC$ | k1_R02RCO3*0.1 | Taraborrelli (2016) |
| G48227 | TrGTerC | $C721CO3H + OH \rightarrow C721CO3$ | 9.65E-12 | Rickard and Pascoe (2009) |
| G48228 | TrGTerC | $NORPINIC + OH \rightarrow C721O2 + CO_2$ | 6.57E-12 | Rickard and Pascoe (2009) |
| G48229 | TrGTerCN | $C721PAN + OH \rightarrow C721OOH + CO + NO_2$ | 2.96E-12 | Rickard and Pascoe (2009) |
| G48230 | TrGTerCN | $C721PAN \rightarrow C721CO3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G48231 | TrGTerC | $C8BC + OH \rightarrow C8BCO2$ | 3.04E-12 | Rickard and Pascoe (2009) |
| G48232 | TrGTerC | $C8BCO2 + HO_2 \rightarrow C8BCOOH$ | KR02HO2(8) | Rickard and Pascoe (2009) |
| G48233a | TrGTerCN | $C8BCO2 + NO \rightarrow C89O2 + NO_2$ | KR02NO*(1.-alpha_AN(8,2,0,0,0, temp, cair)) | Rickard and Pascoe (2009) |
| G48233b | TrGTerCN | $C8BCO2 + NO \rightarrow C8BCNO3$ | KR02NO*alpha_AN(8,2,0,0,0,temp, cair) | Rickard and Pascoe (2009) |
| G48234 | TrGTerC | $C8BCO2 \rightarrow C89O2$ | k1_R02sR02 | Rickard and Pascoe (2009) |
| G48235 | TrGTerC | $C8BCOOH + OH \rightarrow C8BCCO + OH$ | 1.62E-11 | Rickard and Pascoe (2009) |
| G48236 | TrGTerCN | $C8BCNO3 + OH \rightarrow C8BCCO + NO_2$ | 1.84E-12 | Rickard and Pascoe (2009) |
| G48237 | TrGTerC | $C8BCCO + OH \rightarrow C89O2$ | 3.94E-12 | Rickard and Pascoe (2009) |
| G48238 | TrGTerC | $C89O2 + HO_2 \rightarrow C89OOH$ | KR02HO2(8) | Rickard and Pascoe (2009) |
| G48239a | TrGTerCN | $C89O2 + NO \rightarrow C810O2 + NO_2$ | KR02NO*(1.-alpha_AN(7,2,0,0,0, temp, cair)) | Rickard and Pascoe (2009) |
| G48239b | TrGTerCN | $C89O2 + NO \rightarrow C89NO3$ | KR02NO*alpha_AN(7,2,0,0,0,temp, cair) | Rickard and Pascoe (2009) |
| G48240 | TrGTerCN | $C89O2 + NO_3 \rightarrow C810O2 + NO_2$ | KR02NO3 | Rickard and Pascoe (2009) |
| G48241 | TrGTerC | $C89O2 \rightarrow C810O2$ | k1_R02tR02 | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|----------------------------|
| G48242 | TrGTerC | $C89OOH + OH \rightarrow C89O2$ | 3.61E-11 | Rickard and Pascoe (2009) |
| G48243 | TrGTerCN | $C89NO3 + OH \rightarrow CH_3COCH_3 + CO13C4CHO + NO_2$ | 2.56E-11 | Rickard and Pascoe (2009) |
| G48244 | TrGTerC | $C810O2 + HO_2 \rightarrow C810OOH$ | KR02H02(8) | Rickard and Pascoe (2009) |
| G48245a | TrGTerCN | $C810O2 + NO \rightarrow CH_3COCH_3 + C514O2 + NO_2$ | KR02N0*(1.-alpha_AN(10,3,0,0,0, temp, cair)) | Rickard and Pascoe (2009) |
| G48245b | TrGTerCN | $C810O2 + NO \rightarrow C810NO3$ | KR02N0*alpha_AN(10,3,0,0,0, temp, cair) | Rickard and Pascoe (2009) |
| G48246 | TrGTerCN | $C810O2 + NO_3 \rightarrow CH_3COCH_3 + C514O2 + NO_2$ | KR02N03 | Rickard and Pascoe (2009) |
| G48247 | TrGTerC | $C810O2 \rightarrow CH_3COCH_3 + C514O2$ | k1_R02tR02 | Rickard and Pascoe (2009) |
| G48248 | TrGTerC | $C810OOH + OH \rightarrow C810O2$ | 8.35E-11 | Rickard and Pascoe (2009) |
| G48249 | TrGTerCN | $C810NO3 + OH \rightarrow CH_3COCH_3 + CO13C4CHO + NO_2$ | 4.96E-11 | Rickard and Pascoe (2009) |
| G48400a | TrGAroC | $LXYL + OH \rightarrow TLEPOXMUC + HO_2 + LCARBON$ | 0.401E-11 | Rickard and Pascoe (2009)* |
| G48400b | TrGAroC | $LXYL + OH \rightarrow C6H5CH2O2 + LCARBON$ | 0.101E-11 | Rickard and Pascoe (2009)* |
| G48400c | TrGAroC | $LXYL + OH \rightarrow CRESOL + LCARBON$ | 0.261E-11 | Rickard and Pascoe (2009)* |
| G48400d | TrGAroC | $LXYL + OH \rightarrow TLBIPERO2 + HO_2 + LCARBON$ | 0.932E-11 | Rickard and Pascoe (2009)* |
| G48401 | TrGAroCN | $LXYL + NO_3 \rightarrow C6H5CH2O2 + HNO_3 + LCARBON$ | 3.9E-16 | Rickard and Pascoe (2009)* |
| G48402 | TrGAroC | $EBENZ + OH \rightarrow .10 TLEPOXMUC + .07 C6H5CH2O2 + .18 CRESOL + .65 TLBIPERO2 + .28 HO_2 + LCARBON$ | 7.00E-12 | Rickard and Pascoe (2009)* |
| G48403 | TrGAroCN | $EBENZ + NO_3 \rightarrow C6H5CH2O2 + HNO_3 + LCARBON$ | 1.20E-16 | Rickard and Pascoe (2009)* |
| G48404 | TrGAroCN | $STYRENE + NO_3 \rightarrow NSTYRENO2$ | 1.50E-12 | Rickard and Pascoe (2009) |
| G48405 | TrGAroC | $STYRENE + O_3 \rightarrow .545 HCHO + .1 BENZENE + .28 C6H5O2 + .56 CO + .36 OH + .28 HO_2 + .075 PHCOOH + .545 BENZAL + .09 H_2O_2 + .075 HCOOH + .2 CO_2$ | 1.70E-17 | Rickard and Pascoe (2009)* |
| G48406 | TrGAroC | $STYRENE + OH \rightarrow STYRENO2$ | 5.80E-11 | Rickard and Pascoe (2009) |
| G48407 | TrGAroCN | $NSTYRENO2 + HO_2 \rightarrow NSTYRENOOH$ | KR02H02(8) | Rickard and Pascoe (2009) |
| G48408 | TrGAroCN | $NSTYRENO2 + NO \rightarrow NO_2 + NO_2 + HCHO + BENZAL$ | KR02N0 | Rickard and Pascoe (2009)* |
| G48409 | TrGAroCN | $NSTYRENO2 + NO_3 \rightarrow NO_2 + NO_2 + HCHO + BENZAL$ | KR02N03 | Rickard and Pascoe (2009)* |
| G48410 | TrGAroCN | $NSTYRENO2 \rightarrow NO_2 + HCHO + BENZAL$ | k1_R02sR02 | Rickard and Pascoe (2009)* |
| G48411 | TrGAroCN | $NSTYRENOOH + OH \rightarrow NSTYRENO2$ | 6.16E-11 | Rickard and Pascoe (2009) |
| G48412a | TrGAroC | $STYRENO2 + HO_2 \rightarrow STYRENOOH$ | KR02H02(8)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009) |
| G48412b | TrGAroC | $STYRENO2 + HO_2 \rightarrow HO_2 + OH + HCHO + BENZAL$ | KR02H02(8)*rchohch2o2_oh | Rickard and Pascoe (2009)* |
| G48413 | TrGAroCN | $STYRENO2 + NO \rightarrow NO_2 + HO_2 + HCHO + BENZAL$ | KR02N0 | Rickard and Pascoe (2009)* |
| G48414 | TrGAroCN | $STYRENO2 + NO_3 \rightarrow NO_2 + HO_2 + HCHO + BENZAL$ | KR02N03 | Rickard and Pascoe (2009)* |
| G48415 | TrGAroC | $STYRENO2 \rightarrow HO_2 + HCHO + BENZAL$ | k1_R02sR02 | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|---|
| G48416 | TrGAroC | STYRENOOH + OH → STYRENO2 | 6.16E-11 | Rickard and Pascoe (2009) |
| G49200 | TrGTerC | C96O2 → C97O2 | k1_R02pR02 | Rickard and Pascoe (2009) |
| G49201 | TrGTerC | C96O2 + HO ₂ → C96OOH | KR02H02(9) | Rickard and Pascoe (2009) |
| G49202a | TrGTerCN | C96O2 + NO → C97O2 + NO ₂ | KR02N0*(1.-alpha_AN(10,1,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G49202b | TrGTerCN | C96O2 + NO → C96NO3 | KR02N0*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 | 0.6*k_CH300H_OH | Rickard and Pascoe (2009) |
| G49205b | TrGTerC | C96OOH + OH → NORPINAL + OH | 1.30E-11 | Rickard and Pascoe (2009) |
| G49206 | TrGTerC | C97O2 → C98O2 | k1_R02tR02 | Rickard and Pascoe (2009) |
| G49207 | TrGTerCN | C97O2 + NO → C98O2 + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G49208a | TrGTerC | C97O2 + HO ₂ → C97OOH | KR02H02(9)*rcoch2o2_ooH | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G49208b | TrGTerC | C97O2 + HO ₂ → C98O2 + OH | KR02H02(9)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G49209 | TrGTerC | C97OOH + OH → C97O2 | 1.05E-11 | Rickard and Pascoe (2009) |
| G49210 | TrGTerC | C98O2 → C614O2 + CH ₃ COCH ₃ | k1_R02tR02 | Rickard and Pascoe (2009) |
| G49211a | TrGTerCN | C98O2 + NO → C614O2 + CH ₃ COCH ₃ + NO ₂ | KR02N0*(1.-alpha_AN(12,3,0,0,0, temp,cair)) | Rickard and Pascoe (2009) |
| G49211b | TrGTerCN | C98O2 + NO → 9 LCARBON + LNITROGEN | KR02N0*alpha_AN(12,3,0,0,0, temp,cair) | Rickard and Pascoe (2009) |
| G49212 | TrGTerC | C98O2 + HO ₂ → C98OOH | KR02H02(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 | KN03AL*8.5 | Rickard and Pascoe (2009) |
| G49216 | TrGTerC | C85CO3 → C85O2 + CO ₂ | k1_R02RC03 | 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_CH3C03_N02 | Rickard and Pascoe (2009) |
| G49219a | TrGTerC | C85CO3 + HO ₂ → C85CO3H | KAPH02*(rco3_ooH+rco3_o3) | Rickard and Pascoe (2009) |
| G49219b | TrGTerC | C85CO3 + HO ₂ → C85O2 + CO ₂ + OH | KAPH02*rco3_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_R02RC03*0.9 | Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|----------------------------|--|
| G49223b | TrGTerC | $C89CO3 \rightarrow C89CO2H$ | $k1_R02RC03*0.1$ | Taraborrelli (2016) |
| G49224a | TrGTerC | $C89CO3 + HO_2 \rightarrow C89CO3H$ | $KAPH02*rc03_ooh$ | Rickard and Pascoe (2009) |
| G49224b | TrGTerC | $C89CO3 + HO_2 \rightarrow C89CO2H + O_3$ | $KAPH02*rc03_o3$ | Rickard and Pascoe (2009) |
| G49224c | TrGTerC | $C89CO3 + HO_2 \rightarrow .80 C811CO3 + .20 C89O2 + .2 CO_2 + OH$ | $KAPH02*rc03_oh$ | Rickard and Pascoe (2009) |
| G49225 | TrGTerCN | $C89CO3 + NO_2 \rightarrow C89PAN$ | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G49226 | TrGTerCN | $C89CO3 + NO \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G49227 | TrGTerC | $C89CO2H + OH \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2$ | $2.69E-11$ | Rickard and Pascoe (2009) |
| G49228 | TrGTerC | $C89CO3H + OH \rightarrow C89CO3$ | $3.00E-11$ | Rickard and Pascoe (2009) |
| G49229 | TrGTerCN | $C89PAN \rightarrow C89CO3 + NO_2$ | k_PAN_M | Rickard and Pascoe (2009) |
| G49230 | TrGTerCN | $C89PAN + OH \rightarrow CH_3COCH_3 + CO13C4CHO + CO + NO_2$ | $2.52E-11$ | Rickard and Pascoe (2009) |
| G49231a | TrGTerC | $C811CO3 \rightarrow C811O2 + CO_2$ | $k1_R02RC03*0.9$ | Taraborrelli (2016) |
| G49231b | TrGTerC | $C811CO3 \rightarrow PINIC$ | $k1_R02RC03*0.1$ | Taraborrelli (2016) |
| G49232a | TrGTerC | $C811CO3 + HO_2 \rightarrow C811CO3H$ | $KAPH02*rc03_ooh$ | Rickard and Pascoe (2009) |
| G49232b | TrGTerC | $C811CO3 + HO_2 \rightarrow PINIC + O_3$ | $KAPH02*rc03_o3$ | Rickard and Pascoe (2009) |
| G49232c | TrGTerC | $C811CO3 + HO_2 \rightarrow C811O2 + CO_2 + OH$ | $KAPH02*rc03_oh$ | Rickard and Pascoe (2009) |
| G49233 | TrGTerCN | $C811CO3 + NO \rightarrow C811O2 + CO_2 + NO_2$ | KAPNO | Rickard and Pascoe (2009) |
| G49234 | TrGTerCN | $C811CO3 + NO_2 \rightarrow C811PAN$ | k_CH3C03_N02 | Rickard and Pascoe (2009) |
| G49235 | TrGTerC | $PINIC + OH \rightarrow C811O2 + CO_2$ | $7.29E-12$ | Rickard and Pascoe (2009) |
| G49236 | TrGTerC | $NOPINONE + OH \rightarrow NOPINDO2$ | $1.55E-11$ | Capouet et al. (2008), Rickard and Pascoe (2009) |
| G49237a | TrGTerC | $NOPINDO2 + HO_2 \rightarrow NOPINDOOH$ | $KR02H02(9)*rc0ch2o2_ooh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G49237b | TrGTerC | $NOPINDO2 + HO_2 \rightarrow C89CO3 + OH$ | $KR02H02(9)*rc0ch2o2_oh$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G49238 | TrGTerCN | $NOPINDO2 + NO \rightarrow C89CO3 + NO_2$ | KR02NO | Rickard and Pascoe (2009)* |
| G49239 | TrGTerC | $NOPINDO2 \rightarrow C89CO3$ | $k1_R02p0R02$ | Rickard and Pascoe (2009) |
| G49240 | TrGTerC | $NOPINDOOH \rightarrow NOPINDCO$ | $2.63E-11$ | Rickard and Pascoe (2009) |
| G49241 | TrGTerC | $NOPINDCO + OH \rightarrow C89CO3$ | $3.07E-12$ | Rickard and Pascoe (2009) |
| G49242 | TrGTerC | $NOPINOO \rightarrow NOPINONE + H_2O_2$ | $6.00E-18*c(ind_H20)$ | Rickard and Pascoe (2009) |
| G49243 | TrGTerC | $NOPINOO + CO \rightarrow NOPINONE + CO_2$ | $1.2E-15$ | Rickard and Pascoe (2009) |
| G49244 | TrGTerCN | $NOPINOO + NO \rightarrow NOPINONE + NO_2$ | $1.E-14$ | Rickard and Pascoe (2009) |
| G49245 | TrGTerCN | $NOPINOO + NO_2 \rightarrow NOPINONE + NO_3$ | $1.E-15$ | Rickard and Pascoe (2009) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|--|
| G49246 | TrGTerC | NORPINENOL + OH → HCOOH + OH + C86O2 | k_CH2CHOH_OH_HCOOH | Taraborrelli (2016), So et al. (2014)* |
| G49247 | TrGTerC | NORPINENOL + HCOOH → NORPINAL + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G49248 | TrGTerC | NORPINAL + HCOOH → NORPINENOL + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (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 | KR02N0*(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), Taraborrelli (2016) |
| G40201b | TrGTerCN | LAPINABO2 + NO → LAPINABNO3 | KR02N0*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40202a | TrGTerC | LAPINABO2 + HO ₂ → LAPINABOOH | KR02H02(10)*(1-rchohch2o2_oh) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40202b | TrGTerC | LAPINABO2 + HO ₂ → PINAL + HO ₂ + OH | KR02H02(10)*rchohch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40203 | TrGTerC | LAPINABO2 → PINAL + HO ₂ | R02*(0.65*k1_R02tOR02+.35*k1_R02sOR02) | 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 | KR02N0 | Vereecken et al. (2007)* |
| G40208 | TrGTerC | OHMENTHEN6ONEO2 + HO ₂ → 2OHMENTHEN6ONE | KR02H02(10) | Vereecken et al. (2007) |
| G40209 | TrGTerC | OHMENTHEN6ONEO2 → 2OHMENTHEN6ONE + HO ₂ | k1_R02tOR02 | Vereecken et al. (2007) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| 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) | T. J. Wallington et al. (2014)* |
| G40212 | TrGTerCN | PINAL + NO ₃ → C96CO3 + HNO ₃ | 2.0E-14 | T. J. Wallington et al. (2014)* |
| G40213a | TrGTerC | C96CO3 → C96O2 + CO ₂ | k1_R02RC03*0.9 | Rickard and Pascoe (2009) |
| G40213b | TrGTerC | C96CO3 → PINONIC | k1_R02RC03*0.1 | Rickard and Pascoe (2009) |
| G40214a | TrGTerC | C96CO3 + HO ₂ → PERPINONIC | KAPH02*rco3_ooh | Rickard and Pascoe (2009) |
| G40214b | TrGTerC | C96CO3 + HO ₂ → PINONIC + O ₃ | KAPH02*rco3_o3 | Rickard and Pascoe (2009) |
| G40214c | TrGTerC | C96CO3 + HO ₂ → C96O2 + OH + CO ₂ | KAPH02*rco3_oh | Rickard and Pascoe (2009) |
| G40215 | TrGTerCN | C96CO3 + NO ₂ → C10PAN2 | k_CH3C03_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 | KR02N03*1.60 | 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 | KR02H02(10) | Rickard and Pascoe (2009) |
| G40223a | TrGTerCN | PINALO2 + NO → C106O2 + NO ₂ | KR02N0*(1.-alpha_AN(12,3,0,1,0, temp, cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40223b | TrGTerCN | PINALO2 + NO → PINALNO3 | KR02N0*alpha_AN(12,3,0,1,0, temp, cair) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40224 | TrGTerC | PINALO2 → C106O2 | k1_R02tR02 | Rickard and Pascoe (2009) |
| G40225 | TrGTerC | PINALOOH + OH → PINALO2 | 2.75E-11 | Rickard and Pascoe (2009) |
| G40226 | TrGTerCN | PINALNO3 + OH → CO235C6CHO + CH ₃ COCH ₃ + NO ₂ | 2.25E-11 | Rickard and Pascoe (2009) |
| G40227 | TrGTerC | C106O2 + HO ₂ → C106OOH | KR02H02(10) | Rickard and Pascoe (2009) |
| G40228a | TrGTerCN | C106O2 + NO → C716O2 + CH ₃ COCH ₃ + NO ₂ | KR02N0*0.875*(1.-alpha_AN(13,3,0,0,0, temp, cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40228b | TrGTerCN | C106O2 + NO → C106NO3 | KR02N0*0.875*alpha_AN(13,3,0,0,0, temp, cair) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40229 | TrGTerC | C106O2 → C716O2 + CH ₃ COCH ₃ | k1_R02tR02 | Rickard and Pascoe (2009) |
| G40230 | TrGTerC | C106OOH + OH → C106O2 | 8.01E-11 | Rickard and Pascoe (2009) |
| G40231 | TrGTerCN | C106NO3 + OH → CO235C6CHO + CH ₃ COCH 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 APINA00 + .44 C109O2 | 8.05E-16*EXP(-640./TEMP) | T. J. Wallington et al. (2014)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|---|
| G40233 | TrGTerC | APINAOO → PINAL + H ₂ O 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) |
| 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 ₂ O 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_R02p0R02 | Rickard and Pascoe (2009) |
| G40242 | TrGTerCN | C109O2 + NO → C89CO3 + HCHO + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G40243a | TrGTerC | C109O2 + HO ₂ → C109OOH | KR02H02(10)*rcoch2o2_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40243b | TrGTerC | C109O2 + HO ₂ → C89CO3 + HCHO + OH | KR02H02(10)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| 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) | T. J. Wallington et al. (2014)* |
| G40247 | TrGTerCN | LNAPINABO2 → PINAL + NO ₂ | (0.65*k1_R02tR02 + 0.35*k1_R02sR02) | Rickard and Pascoe (2009) |
| G40248 | TrGTerCN | LNAPINABO2 + NO → PINAL + NO ₂ + NO ₂ | KR02N0 | Rickard and Pascoe (2009)* |
| G40249 | TrGTerCN | LNAPINABO2 + HO ₂ → LNAPINABOOH | KR02H02(10) | Rickard and Pascoe (2009) |
| G40250 | TrGTerCN | LNAPINABO2 + NO ₃ → PINAL + NO ₂ + NO ₂ | KR02N03 | 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 | KR02H02(10)*rcoch2o2_ooh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40253b | TrGTerC | BPINAO2 + HO ₂ → NOPINONE + HCHO + HO ₂ + OH | KR02H02(10)*rcoch2o2_oh | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40254a | TrGTerCN | BPINAO2 + NO → NOPINONE + HCHO + HO ₂ + NO ₂ | KR02N0*(1.-alpha_AN(11,3,0,0,0, temp, cair)) | Rickard and Pascoe (2009), Taraborrelli (2016) |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| G40254b | TrGTerCN | BPINAO2 + NO → BPINANO3 | KR02NO*alpha_AN(11,3,0,0,0, temp, cair) | Rickard and Pascoe (2009), Taraborrelli (2016) |
| G40255 | TrGTerC | BPINAO2 → NOPINONE + HCHO + HO ₂ | k1_R02t0R02 | Rickard and Pascoe (2009) |
| 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 ₃ COCH ₃ + NO ₂ | KR02NO*(1.-alpha_AN(13,3,0,0,0, temp, cair)) | Vereecken and Peeters (2012) |
| G40258b | TrGTerCN | ROO6R1O2 + NO → ROO6R1NO3 | KR02NO*alpha_AN(13,3,0,0,0, temp, cair) | Vereecken and Peeters (2012) |
| G40259 | TrGTerC | ROO6R1O2 + HO ₂ → 10 LCARBON | KR02HO2(10) | Vereecken and Peeters (2012)* |
| G40260 | TrGTerC | ROO6R1O2 → ROO6R3O2 + CH ₃ COCH ₃ | k1_R02t0R02 | Vereecken and Peeters (2012) |
| G40261a | TrGTerCN | RO6R1O2 + NO → RO6R3O2 + NO ₂ | KR02NO*(1.-alpha_AN(12,3,0,0,0, temp, cair)) | Vereecken and Peeters (2012) |
| G40261b | TrGTerCN | RO6R1O2 + NO → RO6R1NO3 | KR02NO*alpha_AN(12,3,0,0,0, temp, cair) | Vereecken and Peeters (2012) |
| G40262 | TrGTerC | RO6R1O2 + HO ₂ → 10 LCARBON | KR02HO2(10) | Vereecken and Peeters (2012)* |
| G40263 | TrGTerC | RO6R1O2 → RO6R3O2 | k1_R02s0R02 | Vereecken and Peeters (2012) |
| G40264a | TrGTerCN | RO6R3O2 + NO → 9 LCARBON + HCHO + HO ₂ + NO ₂ | KR02NO*(1.-alpha_AN(12,3,0,0,0, temp, cair)) | Vereecken and Peeters (2012) |
| G40264b | TrGTerCN | RO6R3O2 + NO → 10 LCARBON + LNITROGEN | KR02NO*alpha_AN(12,3,0,0,0, temp, cair) | Vereecken and Peeters (2012) |
| G40265 | TrGTerC | RO6R3O2 + HO ₂ → 10 LCARBON | KR02HO2(10) | Vereecken and Peeters (2012) |
| G40266 | TrGTerC | RO6R3O2 → 9 LCARBON + HCHO + HO ₂ | k1_R02sR02 | Vereecken and Peeters (2012)* |
| G40267a | TrGTerC | BPINENE + O ₃ → NOPINONE + .63 CO + .37 CH ₂ OO + .16 OH + .16 HO ₂ | 1.35E-15*EXP(-1270./TEMP) * .051/(1-.027) | T. J. Wallington et al. (2014)* |
| G40267b | TrGTerC | BPINENE + O ₃ → NOPINOO + CO ₂ | 1.35E-15*EXP(-1270./TEMP) * .368/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40267c | TrGTerC | BPINENE + O ₃ → NOPINDO2 + CO ₂ + OH | 1.35E-15*EXP(-1270./TEMP) * .283/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40267d | TrGTerC | BPINENE + O ₃ → C8BC + 2 CO ₂ | 1.35E-15*EXP(-1270./TEMP) * (.104+.167)/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40268 | TrGTerCN | BPINENE + NO ₃ → LNBPINABO2 | 2.51E-12 | T. J. Wallington et al. (2014)* |
| G40269 | TrGTerCN | LNBPINABO2 + HO ₂ → LNBPINABOOH | KR02HO2(10) | Rickard and Pascoe (2009) |
| G40270 | TrGTerCN | LNBPINABO2 + NO → NOPINONE + HCHO + NO ₂ + NO ₂ | KR02NO | Rickard and Pascoe (2009)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|--|
| G40271 | TrGTerCN | LNBPINABO2 + NO ₃ → NOPINONE + HCHO + NO ₂ + NO ₂ | KR02N03 | Rickard and Pascoe (2009) |
| G40272a | TrGTerCN | LNBPINABO2 → NOPINONE + HCHO + NO ₂ | k1_R02tR02*0.7 | Rickard and Pascoe (2009) |
| G40272b | TrGTerCN | LNBPINABO2 → BPINANO3 | k1_R02tR02*0.3 | Rickard and Pascoe (2009) |
| G40273 | TrGTerCN | LNBPINABOOH + OH → LNBPINABO2 | 9.58E-12 | Rickard and Pascoe (2009) |
| G40274 | TrGTerCN | ROO6R1NO3 + OH → ROO6R3O2 + CH ₃ COCH 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 | Taraborrelli (2016), So et al. (2014)* |
| G40277 | TrGTerC | PINEOL + HCOOH → PINAL + HCOOH | k_CH2CHOH_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G40278 | TrGTerC | PINAL + HCOOH → PINEOL + HCOOH | k_ALD_HCOOH | Taraborrelli (2016), daSilva (2010)* |
| G40279a | TrGC | CARENE + OH → LAPINABO2 | 8.7E-11*(.50+.25) | Wolfe et al. (2011), Taraborrelli (2016) |
| G40279b | TrGC | CARENE + OH → MENTHEN6ONE + HO ₂ | 8.7E-11*.25*.60 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40279c | TrGC | CARENE + OH → ROO6R1O2 | 8.7E-11*.25*.40 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40280a | TrGC | CARENE + O ₃ → APINBOO | 2.E-16*.50*.18 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40280b | TrGC | CARENE + O ₃ → PINONIC | 2.E-16*.50*.16 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40280c | TrGC | CARENE + O ₃ → OH + NORPINAL + CO + HO ₂ | 2.E-16*.50*.66 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40280d | TrGC | CARENE + O ₃ → APINAOO | 2.E-16*.50*.12 | Wolfe et al. (2011), Taraborrelli (2016) |
| G40280e | TrGC | CARENE + O ₃ → OH + C109O2 | 2.E-16*.50*(.22+.66) | Wolfe et al. (2011), Taraborrelli (2016) |
| G40281 | TrGCN | CARENE + NO ₃ → LNAPINABO2 | 9.5E-12 | Wolfe et al. (2011), Taraborrelli (2016) |
| 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)* |

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

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|---|---|
| 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 ₂ OOH + .16 OH + .16 HO ₂ | 1.35E-15*EXP(-1270./TEMP) *.051/(1-.027) | T. J. Wallington et al. (2014)* |
| G40283b | TrGTerC | SABINENE + O ₃ → NOPINOO + CO ₂ | 1.35E-15*EXP(-1270./TEMP) *.368/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40283c | TrGTerC | SABINENE + O ₃ → NOPINDO2 + CO ₂ + OH | 1.35E-15*EXP(-1270./TEMP) *.283/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40283d | TrGTerC | SABINENE + O ₃ → C8BC + 2 CO ₂ | 1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40284 | TrGTerCN | SABINENE + NO ₃ → LNBPINABO2 | 2.51E-12 | T. J. Wallington et al. (2014)* |
| 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 ₂ OOH + .16 OH + .16 HO ₂ | 1.35E-15*EXP(-1270./TEMP) *.051/(1-.027) | T. J. Wallington et al. (2014)* |
| G40286b | TrGTerC | CAMPHENE + O ₃ → NOPINOO + CO ₂ | 1.35E-15*EXP(-1270./TEMP) *.368/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40286c | TrGTerC | CAMPHENE + O ₃ → NOPINDO2 + CO ₂ + OH | 1.35E-15*EXP(-1270./TEMP) *.283/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40286d | TrGTerC | CAMPHENE + O ₃ → C8BC + 2 CO ₂ | 1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027) | Nguyen et al. (2009), T. J. Wallington et al. (2014) |
| G40287 | TrGTerCN | CAMPHENE + NO ₃ → LNBPINABO2 | 2.51E-12 | T. J. Wallington et al. (2014)* |
| 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)* |
| G9200 | StTrGS | SO ₂ + OH → H ₂ SO ₄ + HO ₂ | k_3rd(temp, cair, 3.3E-31, 4.3, 1.6E-12, 0., 0.6) | Sander et al. (2011) |
| G9400a | TrGCS | DMS + OH → CH ₃ SO ₂ + HCHO | 1.13E-11*EXP(-253./temp) | Atkinson et al. (2004)* |
| G9400b | TrGCS | DMS + OH → DMSO + HO ₂ | k_DMS_OH | Atkinson et al. (2004)* |
| G9401 | TrGCNS | DMS + NO ₃ → CH ₃ SO ₂ + HNO ₃ + HCHO | 1.9E-13*EXP(520./temp) | Atkinson et al. (2004) |

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

| # | labels | reaction | rate coefficient | reference |
|----------|----------|--|--|--|
| G9402 | TrGCS | $\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$ | 1.E-10 | Hynes and Wine (1996) |
| G9403 | TrGS | $\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3$ | $1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$ | Barone et al. (1995) |
| G9404 | TrGS | $\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$ | 3.E-13 | Barone et al. (1995) |
| G9405 | TrGS | $\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$ | 5.E-11 | Barone et al. (1995) |
| G9408 | StTrGS | $\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$ | k_CH2OO_S02 | Welz et al. (2012), Stone et al. (2014)* |
| G9409 | TrGTerCS | $\text{NOPINOO} + \text{SO}_2 \rightarrow \text{NOPINONE} + \text{H}_2\text{SO}_4$ | 7.E-14 | Rickard and Pascoe (2009) |
| G9410 | TrGTerCS | $\text{APINAOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G9411 | TrGTerCS | $\text{APINBOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G9412 | TrGTerCS | $\text{MBOOO} + \text{SO}_2 \rightarrow \text{IBUTALOH} + \text{H}_2\text{SO}_4$ | 7.00E-14 | Rickard and Pascoe (2009) |
| G0070dCM | StTrG | $\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH}$ | 4.0/(680*100) | see general notes* |
| G0055dUJ | StTrGC | $\text{C511OOH} \rightarrow \text{C511OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0056dUJ | StTrGC | $\text{C512OOH} \rightarrow \text{C512OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0057dUJ | StTrGC | $\text{C513OOH} \rightarrow \text{C513OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0026dUJ | StTrGC | $\text{ISOPBOOH} \rightarrow \text{ISOPBOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0028dUJ | StTrGC | $\text{ISOPDOOH} \rightarrow \text{ISOPDOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0024dUJ | StTrGC | $\text{C59OOH} \rightarrow \text{C59OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0070dUJ | StTrGC | $\text{C85OOH} \rightarrow \text{C85OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0071dUJ | StTrGC | $\text{C86OOH} \rightarrow \text{C86OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0068dUJ | StTrGC | $\text{C812OOH} \rightarrow \text{C812OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0069dUJ | StTrGC | $\text{C813OOH} \rightarrow \text{C813OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0076dUJ | StTrGC | $\text{C96OOH} \rightarrow \text{C96OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0077dUJ | StTrGC | $\text{C97OOH} \rightarrow \text{C97OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0079dUJ | StTrGC | $\text{C98OOH} \rightarrow \text{C98OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0124dUJ | StTrGC | $\text{PINALOOH} \rightarrow \text{PINALOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0044dUJ | StTrGC | $\text{C106OOH} \rightarrow \text{C106OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0042dUJ | StTrGC | $\text{BPINAOOH} \rightarrow \text{BPINAOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0045dUJ | StTrGC | $\text{C109OOH} \rightarrow \text{C109OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0009dUJ | StTrG | $\text{HCOOH} \rightarrow \text{HCOOHDummy}$ | 0.3/(680*100) | see general notes* |
| G0010dUJ | StTrG | $\text{HOCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0011dUJ | StTrGC | $\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{OOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0081dUJ | StTrGC | $\text{CH}_3\text{CHOHOOH} \rightarrow \text{CH}_3\text{CHOHOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0121dUJ | StTrGC | $\text{NOPINDOOH} \rightarrow \text{NOPINDOOHDummy}$ | 4.0/(680*100) | see general notes* |
| G0074dUJ | StTrGC | $\text{C8BCOOH} \rightarrow \text{C8BCOOHDummy}$ | 4.0/(680*100) | see general notes* |

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

| # | labels | reaction | rate coefficient | reference |
|----------|---------|---|------------------|--------------------|
| G0062dUJ | StTrGC | C721OOH → C721OOHDummy | 4.0/(680*100) | see general notes* |
| G0064dUJ | StTrGC | C722OOH → C722OOHDummy | 4.0/(680*100) | see general notes* |
| G0085dUJ | StTrGC | CO235C6OOH → CO235C6OOHDummy | 4.0/(680*100) | see general notes* |
| G0060dUJ | StTrGC | C614OOH → C614OOHDummy | 4.0/(680*100) | see general notes* |
| G0052dUJ | StTrGC | C413COOOH → C413COOOHDummy | 4.0/(680*100) | see general notes* |
| G0053dUJ | StTrGC | C44OOH → C44OOHDummy | 4.0/(680*100) | see general notes* |
| G0021dUJ | StTrGC | MACROOH → MACROOHDummy | 4.0/(680*100) | see general notes* |
| G0083dUJ | StTrGC | CHOC3COOOH → CHOC3COOOHDummy | 4.0/(680*100) | see general notes* |
| G0094dUJ | StTrGC | LAPINABOOH → LAPINABOOHDummy | 4.0/(680*100) | see general notes* |
| G0013dUJ | StTrGCN | PAN → PANDummy | 0.2/(680*100) | see general notes* |
| G0005dUJ | StTrGN | NO ₃ → NO ₃ Dummy | 4/(680*100) | see general notes* |
| G0006dUJ | StTrGN | HNO ₃ → HNO ₃ Dummy | 4/(680*100) | see general notes* |
| G3116uj | StTrGC | MVK → MVKDummy | 1/(680*100) | see general notes* |
| G3116ujb | StTrGC | MACR → MACRDummy | 1/(680*100) | see general notes* |
| G3119uj | StTrGC | PINAL → PINALDummy | 0.6/(680*100) | see general notes* |

General notes

Three-body reactions

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

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

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

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (3)$$

$$\mathbf{k_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right) \quad (4)$$

A similar function, called `k_3rd_iupac` here, is used by T. J. Wallington et al. (2014) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \quad (8)$$

$$\mathbf{k_3rd_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right) \quad (9)$$

RO₂ 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 described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{1\text{st}} = 2 \times \sqrt{k_{\text{self}} \times k_{\text{CH3O2}}} \times [\text{RO}_2]$ where k_{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 CH₃O₂, and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Deposition of peroxides

The value of 4.0/(680*100) is based on deposition velocities for peroxides obtained by ?. The PBL height of 680 m is based on 120 hour FlexPart (<https://www.flexpart.eu>) backtrajectory simulations. The deposition of PAN is based on ?.

Specific notes

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))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

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.E-30, 4.4, 1.4E-12, 0.7, 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, 1.8E-31, 3.2, 4.7E-12, 1.4, 0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ (1./ (6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)))`

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

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).

G4116: Same value as for PAN + OH.

G4126: Same as for G4104 but scaled to match the recommended 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 CH₃OH can be excluded because of a likely high energy barrier (L. Vereecken, pers. comm.). CH₂OO 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 CH₂OO + NO₂ (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: $\text{HOOCH}_2\text{OCHO}$ 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 .

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of $\text{CH}_3\text{O}_2\text{NO}_2$.

G4150: Value for $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH}$, H-abstraction enhanced by the HO-group by f_{soh} .

G4154: Products assumed to be $\text{CH}_3\text{O}_2 + \text{O}_2$ (could also be $\text{HCHO} + \text{O}_2 + \text{OH}$).

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: $k_{\text{CH3CO3_NO2}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

G42018: The rate coefficient is the same as for the CH_3 channel in G4107 ($\text{CH}_3\text{OOH} + \text{OH}$).

G42021: The rate coefficient is $k_{\text{PAN_M}} = k_{\text{CH3CO3_NO2}}/9.5\text{E-}29 \cdot \exp(-14000./\text{temp})$, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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 $\text{HOCH}_2\text{CH}_2\text{O}$ in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are $2 \text{HCHO} + \text{HO}_2$.

G42051a: Same as for the CH_3O_2 channel in G4107: $\text{CH}_3\text{OOH} + \text{OH}$.

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

G42074a: Factor of 3 to match the estimate of $k = 1.1\text{E-}11 \text{ molec/cm}^3/\text{s}$ by Paulot et al. (2009a).

G42074b: Factor of 3 to match the estimate of $k = 1.1\text{E-}11 \text{ molec/cm}^3/\text{s}$ by Paulot et al. (2009a).

G42075: $\text{NO}_3\text{CH}_2\text{CO}_2\text{H}$ and $\text{NO}_3\text{CH}_2\text{CO}_3\text{H}$ neglected.

G42078: $\text{NO}_3\text{CH}_2\text{CO}_2\text{H}$ 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, $\text{OH} + \text{HCHO} + \text{HOCN}$, could not be confirmed by Tyndall et al. (2001b). There is no alternative mechanism at the moment. Products assumed to be $\text{OH} + \text{CH}_3\text{CO}_3 + \text{NO}$

G42086b: Assuming HCN is from channel 2h, $\text{HCO} + \text{H} + \text{HCN}$. HCO is replaced by $\text{H} + \text{CO}$.

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

G42087: HCOCN is produced but replaced here by its likely oxidation products ($\text{HCN} + \text{CO}_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $\text{RO}_2 + \text{NO}$ reaction is used.

G42088: NCCH_2OOH is produced but replaced here by its likely oxidation products ($\text{HCN} + \text{CO}_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $\text{RO}_2 + \text{HO}_2$ reaction is used.

G42089a: The minor channel with $k=5.2\text{E-}12$ 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).

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

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

G43004: The value for the generic $\text{RO}_2 + \text{HO}_2$ reaction from Atkinson (1997) is used here.

G43008: The value for the generic $\text{RO}_2 + \text{HO}_2$ reaction from Atkinson (1997) is used here.

G43011: Strong positive deviation of k below 240 K compared to the expression recommended by JPL (Sander et al., 2011).

G43015a: The same value as for G4107 ($\text{CH}_3\text{OOH} + \text{OH}$) 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 $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH}$, H-abstraction enhanced by the CH_3CO -group by f_{co} .

G43051c: Products approximated with $\text{C}_2\text{H}_5\text{CHO} + \text{HO}_2$.

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 $\text{CHCH}(\text{OH})_2$.

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.

G43223: Products simplified

G43419: $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

G43420: $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

G43421: Permutation reaction (minor channels removed).

G44000: The $\text{LC}_4\text{H}_9\text{O}_2$ composition ($n\text{C}_4\text{H}_9\text{O}_2:s\text{C}_4\text{H}_9\text{O}_2$ ratio) is assumed to be equal to the ratio of the production rates at 298K: $k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}) = 0.1273$ and $k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}) = 0.8727$.

G44001b: $s\text{C}_4\text{H}_9\text{O}_2$ products are substituted with 0.636 MEK + HO_2 and 0.364 $\text{CH}_3\text{CHO} + \text{C}_2\text{H}_5\text{O}_2$ at 1 bar and 298 K.

G44003c: The alkyl nitrate yield is the weighted average yield for the two isomers forming from $n\text{C}_4\text{H}_9\text{O}_2$ and $s\text{C}_4\text{H}_9\text{O}_2$.

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 -ONO₂ 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 $\text{HCHO} + \text{CO}_2 + \text{HOCH}_2\text{CH}_2\text{O}_2$.

G44023a: Products from H-abstraction from the tertiary carbon bearing the ONO₂ group.

G44023b: Products from H-abstraction from the secondary carbon bearing the ONO₂ 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 RO₂.

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 RO₂ is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO2 isomers mostly C₂H₅CHO.

G44097a: Branching ratios according to Rickard et al. (1999). CH₃CHO₂CHO is replaced with its major products CH₃CHO + CO + HO₂.

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

G44098: The nitrated RO₂ 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 C₃H₆ + O₃ reaction.

G44107: The nitrated RO₂ is replaced by its products upon reaction with NO.

G44110: The nitrated RO₂ 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 → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44407: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44409: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44410: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44412: KDEC BZFUONOOA → .5 BZFUONOO + .5 CO + .5 CO₂ + .5 HCOCH₂O₂ + .5 OH and BZFUONOO → .625 CO₁₄O₃CO₂H + .375 CO₁₄O₃CHO + .375 H₂O

G44421: Only major channel.

G44424: KDEC: GLYOOA → .125 HCHO + .18 GLYOO + 0.82 HO₂ + .57 OH + 1.265 CO + .25 CO₂ and H₂O substitution GLYOO → .625 HCOCO₂H + .375 GLYOX + .375 H₂O

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCOC₃

G44431: KDEC MALANHYO → HCOCOHCOC₃

G44432: Only major channel. KDEC MALANHYO → HCOCOHCOC₃

G44436: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂

G44437: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂

G44438: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂ and RO₂ Only major channel.

G44439: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .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 \rightarrow GLYOX + GLYOX + HO2

G44458: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2

G44459: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2. Only major channel.

G44461: KBPAN \rightarrow 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: ZCODC23DBCOD = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with NO₃ 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 HO₂ 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 RO₂-to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with O₂ forming HCOOH + HO₂. Along CH₃COCHOOHCHO should be produced but not in the mechanism. Only CH₃COCHO₂CHO. 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 RO₂ that upon conversion to RO yields 100% 2-methyl-butenedial (ZCODC23DBCOD) although Aschmann et al. (2014) quantified a 38% yield of the Z/E mixture.

G45129: As for 3METHYLFURAN + OH but with additional NO₂ 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: ZCPANC23DBCOD 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 = .67 MBOAO2 + .33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2 \rightarrow MMALANHY + NO2

G45404: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45405: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45406: KDEC NTLFUO \rightarrow ACCOMECHO

G45409: KBPAN \rightarrow 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 →.83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45431: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45432: KFPAN →k.CH3CO3_NO2 (renaming)

G45433: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45434: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2 and only major channel.

G45436: KDEC C5CO14CO2 → .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45444: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3 + .35 CO + .35 CO2 + .65 MMALANHY + .65 HO2

G45452: KDEC TLFUONOOA →.5 CO + .5 OH + .5 MECOACETO2 + .5 TLFUONOO and H2O subs TLFUONOO →.625 C24O3CCO2H + .375 ACCOMECHO + .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 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

G46462: KDEC PHENO \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

G46463: KDEC PHENO \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

G46464: KDEC PHENO \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2 and Only major channel.

G46468: KFPAN \rightarrow k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO \rightarrow C5CO2OHCO3

G46481: KDEC PBZQO \rightarrow C5CO2OHCO3

G46482: KDEC PBZQO \rightarrow C5CO2OHCO3

G46483: KDEC PBZQO \rightarrow C5CO2OHCO3 and Only major channel.

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

G46486: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46490b: Reactions with KRO2HO2 and KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO.

G46491b: KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO.

G46492: KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

G46493: KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO and Only major channel.

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

G46500: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46501: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46502: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

G46517b: New channel.

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

G46523b: KDEC BZBIPERO \rightarrow GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

G46524: KDEC BZBIPERO \rightarrow GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

G46525: KDEC BZBIPERO \rightarrow GLYOX + HO2 + .5 BZFUONE + .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 with its oxidation product BENZAL.

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero2_oh is set to 0.40 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

G47408a: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47408b: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DB COD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47409: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DB COD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47410: Only major channel and KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DB COD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47412: KDEC MGLOOB \rightarrow .125 CH3CHO + .695 CH3CO + .57 CO + .57 OH + .125 HO2 + .18 MGLOO + .25 CO2

G47413: Merged.

G47418b: Reactions with KRO2HO2 and KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE.

G47419: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

G47420: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

G47421: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE and Only major channel.

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

G47423: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

G47429: KDEC MCATECOOA \rightarrow MC3ODBCO2H + HCOCO2H + HO2 + OH

G47436: KFPAN \rightarrow k_CH3CO3_NO2

G47438: Only major channel.

G47439b: Reactions with KRO2HO2 and KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47440b: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47441: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47442: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2 and Only major channel.

G47445: KFPAN \rightarrow k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

G47482b: Reactions with KRO2HO2 and KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47483: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47484: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47485: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO \rightarrow C6CO2OHCO3

G47487: KDEC PTLQO \rightarrow C6CO2OHCO3

G47488: KDEC PTLQO \rightarrow C6CO2OHCO3

G47489: Only major channel. KDEC PTLQO \rightarrow C6CO2OHCO3.

G47494: New channel.

G47497b: Reactions with KRO2HO2 and KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47498: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

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

G47502: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

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

G47510: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47511: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47512: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

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

G47514: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO \rightarrow 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 \rightarrow .24 CH2OO + .40 CO + .36 HO2 + .36 CO + .36 OH and H2Osubs PHCHOO \rightarrow .625 PHCOOH + .375 BENZAL + .375 H2O2 + .2 CO2

G48408: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48409: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48410: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

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

G48413: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

G48414: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

G48415: KDEC STYRENO \rightarrow 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). LAP-INABO2 = .65 APINAO2 + .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).

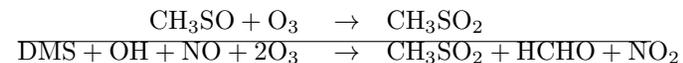
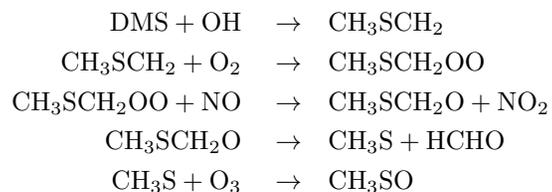
G40286a: Products from Nguyen et al. (2009).

G40287: Products from Rickard and Pascoe (2009).

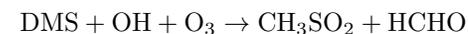
G40400: DIET35TOL(from MCM) as representative of higher aromatics

G40401: Same products as for toluene.

G9400a: For the abstraction path, the assumed reaction sequence (omitting H₂O and O₂ as products) according to Yin et al. (1990) is:



Neglecting the effect on O₃ and NO_x, the remaining reaction is:



G9400b: For the addition path, the rate coefficient is: $k_{\text{DMS_OH}} = 1.0\text{E-}39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{ind_02}) / (1.+5.0\text{E-}30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{ind_02}))$.

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

Table 2: Photolysis reactions

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|--|----------------------|---|
| J1000a | UpStTrGJ | $O_2 + h\nu \rightarrow O(^3P) + O(^3P)$ | jx(ip_02) | Sander et al. (2014) |
| J1001a | UpStTrGJ | $O_3 + h\nu \rightarrow O(^1D) + O_2$ | jx(ip_01D) | Sander et al. (2014) |
| J1001b | UpStTrGJ | $O_3 + h\nu \rightarrow O(^3P) + O_2$ | jx(ip_03P) | Sander et al. (2014) |
| J2101 | UpStTrGJ | $H_2O_2 + h\nu \rightarrow 2 OH$ | jx(ip_H2O2) | Sander et al. (2014) |
| J3101 | UpStTrGJN | $NO_2 + h\nu \rightarrow NO + O(^3P)$ | jx(ip_N02) | Sander et al. (2014) |
| J3103a | UpStTrGJN | $NO_3 + h\nu \rightarrow NO_2 + O(^3P)$ | jx(ip_N020) | Sander et al. (2014) |
| J3103b | UpStTrGJN | $NO_3 + h\nu \rightarrow NO + O_2$ | jx(ip_N002) | Sander et al. (2014) |
| J3104 | StTrGJN | $N_2O_5 + h\nu \rightarrow NO_2 + NO_3$ | jx(ip_N205) | 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_HN03) | Sander et al. (2014) |
| J3202 | StTrGJN | $HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$ | jx(ip_HN04) | Sander et al. (2014) |
| J41000 | StTrGJ | $CH_3OOH + h\nu \rightarrow CH_3O + OH$ | jx(ip_CH300H) | Sander et al. (2014) |
| J41001a | StTrGJ | $HCHO + h\nu \rightarrow H_2 + CO$ | jx(ip_COH2) | Sander et al. (2014) |
| J41001b | StTrGJ | $HCHO + h\nu \rightarrow H + CO + HO_2$ | jx(ip_CHOH) | Sander et al. (2014) |
| J41004 | StTrGJN | $CH_3ONO + h\nu \rightarrow CH_3O + NO$ | jx(ip_CH30NO) | 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_CH300H) | Sander et al. (2014) |
| J41008 | StTrGJ | $CH_3O_2 + h\nu \rightarrow HCHO + OH$ | jx(ip_CH302) | 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_CH300H) | 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), Sander et al. (2011) |
| J42005a | TrGJC | $HOCH_2CHO + h\nu \rightarrow HCHO + 2 HO_2 + CO$ | jx(ip_HOCH2CHO)*0.83 | Sander et al. (2011) |
| J42005b | TrGJC | $HOCH_2CHO + h\nu \rightarrow OH + HCOCH_2O_2$ | jx(ip_HOCH2CHO)*0.07 | Sander et al. (2011) |
| J42005c | TrGJC | $HOCH_2CHO + h\nu \rightarrow CH_3OH + CO$ | jx(ip_HOCH2CHO)*0.10 | Sander et al. (2011) |
| J42006 | TrGJC | $HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$ | jx(ip_CH300H) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|--------|----------|--|---|--------------------------------|
| J42007 | TrGJCN | PHAN + $h\nu$ → .7 HOCH ₂ CO + .7 NO ₂ + .3 HCHO + .3 HO ₂ + .3 CO ₂ + .3 NO ₃ | jx(ip_PAN) | see note* |
| J42008 | TrGJC | GLYOX + $h\nu$ → 2 CO + 2 HO ₂ | jx(ip_GLYOX) | Sander et al. (2014) |
| J42009 | TrGJC | HCOCO ₂ H + $h\nu$ → 2 HO ₂ + CO + CO ₂ | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J42010 | TrGJC | HCOCO ₃ H + $h\nu$ → HO ₂ + CO + OH + CO ₂ | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J42011 | TrGJC | HYETHO ₂ H + $h\nu$ → HOCH ₂ CH ₂ O + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J42012 | TrGJCN | ETHOHNO ₃ + $h\nu$ → HO ₂ + 2 HCHO + NO ₂ | J_IC3H7N03 | Rickard and Pascoe (2009) |
| J42013 | TrGJC | HOOCH ₂ CO ₃ H + $h\nu$ → OH + HCHO + CO ₂ + OH | 2*jx(ip_CH300H) | Taraborrelli (2016) |
| J42014 | TrGC | HOOCH ₂ CO ₂ H + $h\nu$ → OH + HCHO + HO ₂ + CO ₂ | jx(ip_CH300H) | Taraborrelli (2016) |
| J42015 | TrGC | CH ₂ CO + $h\nu$ → .4 CO ₂ + .8 H + .34 CO + .34 OH + .34 HO ₂ + .16 HCHO + .16 O(³ P) + .1 HCOOH + CO | J_ketene* 0.36 | Taraborrelli (2016) |
| J42016 | TrGC | CH ₃ CHOHO ₂ + $h\nu$ → CH ₃ + HCOOH + OH | jx(ip_CH300H) | Taraborrelli (2016) |
| J42017 | TrGJCN | NO ₃ CH ₂ CHO + $h\nu$ → HO ₂ + CO + HCHO + NO ₂ | (jx(ip_C2H5N03)+jx(ip_CH3CHO)) *(jx(ip_NOA)+1E-10)/(0.59*J_ IC3H7N03+jx(ip_CH3COCH3)+1E-10) | Taraborrelli (2016)* |
| J42018 | TrGJC | HOOCH ₂ CHO + $h\nu$ → OH + HCHO + CO + HO ₂ | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Taraborrelli (2016) |
| J42019 | TrGJCN | C ₂ H ₅ ONO ₂ + $h\nu$ → CH ₃ CHO + HO ₂ + NO ₂ | jx(ip_C2H5N03) | Taraborrelli (2016) |
| J42020 | TrGJCN | NO ₃ CH ₂ CHO + $h\nu$ → .7 NO ₃ CH ₂ CO ₃ + .7 NO ₂ + .3 HCHO + .3 NO ₂ + .3 CO ₂ + .3 NO ₃ | jx(ip_PAN) | Taraborrelli (2016)* |
| J42021 | StTrGJCN | C ₂ H ₅ O ₂ NO ₂ + $h\nu$ → .667 NO ₂ + .667 C ₂ H ₅ O ₂ + .333 NO ₃ + .333 CH ₃ CHO + .333 HO ₂ | jx(ip_CH302N02) | Taraborrelli (2016)* |
| J43000 | TrGJC | iC ₃ H ₇ OOH + $h\nu$ → CH ₃ COCH ₃ + HO ₂ + OH | jx(ip_CH300H) | von Kuhlmann (2001) |
| J43001 | TrGJC | CH ₃ COCH ₃ + $h\nu$ → CH ₃ C(O) + CH ₃ | jx(ip_CH3COCH3) | Sander et al. (2014) |
| J43002 | TrGJC | CH ₃ COCH ₂ OH + $h\nu$ → .5 CH ₃ C(O) + .5 HCHO + .5 HO ₂ + .5 HOCH ₂ CO + .5 CH ₃ | J_ACETOL | Sander et al. (2011)* |
| J43003 | TrGJC | MGLYOX + $h\nu$ → CH ₃ C(O) + CO + HO ₂ | jx(ip_MGLYOX) | Sander et al. (2014) |
| J43004 | TrGJC | CH ₃ COCH ₂ O ₂ H + $h\nu$ → CH ₃ C(O) + HCHO + OH | jx(ip_CH300H)+J_ACETOL | Rickard and Pascoe (2009) |
| J43005 | TrGJC | HOCH ₂ COCH ₂ O ₂ H + $h\nu$ → HOCH ₂ CO + HCHO + OH | jx(ip_CH300H)+J_ACETOL | Taraborrelli (2016) |
| J43006 | TrGJCN | iC ₃ H ₇ ONO ₂ + $h\nu$ → CH ₃ COCH ₃ + NO ₂ + HO ₂ | J_IC3H7N03 | von Kuhlmann et al. (2003)* |
| J43007 | TrGJCN | NOA + $h\nu$ → CH ₃ C(O) + HCHO + NO ₂ | jx(ip_NOA) | Barnes et al. (1993) |
| J43009 | TrGJC | HYPROPO ₂ H + $h\nu$ → CH ₃ CHO + HCHO + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J43010 | TrGJCN | PR ₂ O ₂ HNO ₃ + $h\nu$ → NOA + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J43011 | TrGJC | HOCH ₂ COCHO + $h\nu$ → HOCH ₂ CO + CO + HO ₂ | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J43012 | TrGJC | HCOCOCH ₂ O ₂ H + $h\nu$ → HCOCO + HCHO + OH | jx(ip_CH300H)+J_ACETOL | Taraborrelli (2016) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|---|--|
| J43013 | TrGJC | $\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$ | $\text{jx}(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J43014 | TrGJTerC | $\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$ | Rickard and Pascoe (2009) |
| J43015 | TrGJTerC | $\text{HCOCH}_2\text{CO}_2\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{HO}_2$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO})$ | Rickard and Pascoe (2009) |
| J43016 | TrGJTerC | $\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009) |
| J43017 | TrGJC | $\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$ | $2 * \text{jx}(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J43018 | TrGJC | $\text{CH}_3\text{COCO}_2\text{H} + h\nu \rightarrow .32 \text{CH}_3\text{CHO} + .16 \text{CH}_2\text{CHOH} + .54 \text{CO}_2$ $+ .38 \text{CH}_3\text{C}(\text{O}) + .38 \text{HO}_2 + .38 \text{CO}_2 + .07 \text{CH}_3\text{COOH} + .07$ $\text{CO} + .05 \text{CH}_3\text{C}(\text{O}) + .05 \text{CO} + .05 \text{OH}$ | $\text{JX}(\text{IP_CH}_3\text{COCOC}_2\text{H})$ | Sander et al. (2011), Taraborrelli (2016)* |
| J43019 | TrGC | $\text{CH}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{CO}_2$ | $\text{JX}(\text{IP_MGLYOX}) + \text{jx}(\text{ip_CH}_3\text{OOH})$ | Taraborrelli (2016) |
| J43020 | TrGC | $\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$ | $\text{J_ketene} * 0.36 * 2.$ | Taraborrelli (2016) |
| J43021 | TrGCN | $\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$ | $\text{J_IC}_3\text{H}_7\text{NO}_3$ | Taraborrelli (2016) |
| J43022 | TrGCN | $\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$ | $\text{jx}(\text{ip_CH}_3\text{O}_2\text{NO}_2) + \text{jx}(\text{ip_CH}_3\text{COCH}_3)$ | Taraborrelli (2016) |
| J43023 | TrGJC | $\text{C}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | von Kuhlmann (2001) |
| J43024 | TrGJCN | $\text{C}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{NO}_2 + \text{HO}_2$ | $0.59 * \text{J_IC}_3\text{H}_7\text{NO}_3$ | see note* |
| J43025a | TrGJC | $\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{HCO})$ | see note* |
| J43025b | TrGJC | $\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$ | Andrews et al. (2012), Taraborrelli (2016)* |
| J43026 | TrGJCN | $\text{PPN} + h\nu \rightarrow .7 \text{C}_2\text{H}_5\text{CO}_3 + .7 \text{NO}_2 + .3 \text{C}_2\text{H}_5\text{O}_2 + .3 \text{CO}_2 +$ $.3 \text{NO}_3$ | $\text{jx}(\text{ip_PAN})$ | Sander et al. (2014), Sander et al. (2011) |
| J43027 | TrGJC | $\text{C}_2\text{H}_5\text{CO}_3\text{H} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | von Kuhlmann (2001) |
| J43028a | TrGJC | $\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$ | $\text{jx}(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J43028b | TrGJC | $\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH}_3\text{OOH})$ | Taraborrelli (2016) |
| J43200 | TrGJTerC | $\text{HCOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009) |
| J43400 | TrGJAroC | $\text{C}_3\text{DIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2 + \text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J43401 | TrGJAroC | $\text{C}_3\text{OH}_3\text{CO} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2$ | Rickard and Pascoe (2009) |
| J43402 | TrGJAroC | $\text{HCOCOHC}_3\text{H} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009) |
| J44000a | TrGJC | $\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$ | $\text{jx}(\text{ip_CH}_3\text{OOH}) * (\text{k}_p / (\text{k}_p + \text{k}_s))$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J44000b | TrGJC | $\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{MEK} + .636 \text{HO}_2 + .364$ $\text{CH}_3\text{CHO} + .364 \text{C}_2\text{H}_5\text{O}_2$ | $\text{jx}(\text{ip_CH}_3\text{OOH}) * (\text{k}_s / (\text{k}_p + \text{k}_s))$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J44001 | TrGJC | $\text{MVK} + h\nu \rightarrow .5 \text{C}_3\text{H}_6 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + \text{CO} + .5$ HO_2 | $\text{jx}(\text{ip_MVK})$ | Sander et al. (2014) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|----------|---|--|---|
| J44002 | TrGJC | $\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$ | $0.42 \cdot jx(\text{ip_CHOH})$ | von Kuhlmann et al. (2003) |
| J44003 | TrGJC | $\text{LMEKOOH} + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$ | $jx(\text{ip_CH300H}) + 0.42 \cdot jx(\text{ip_CHOH})$ | Taraborrelli (2016) |
| J44004 | TrGJC | $\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C}(\text{O})$ | $2.15 \cdot jx(\text{ip_MGLYOX})$ | see note* |
| J44005a | TrGJCN | $\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$ | $\text{J_IC3H7N03} * (\text{k_p} / (\text{k_p} + \text{k_s}))$ | see note* |
| J44005b | TrGJCN | $\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$ | $\text{J_IC3H7N03} * (\text{k_s} / (\text{k_p} + \text{k_s}))$ | see note* |
| J44006 | TrGJCN | $\text{MPAN} + h\nu \rightarrow .7 \text{MACO}_3 + .7 \text{NO}_2 + .3 \text{MACO}_2 + .3 \text{NO}_3$ | $jx(\text{ip_PAN})$ | see note* |
| J44007a | TrGJC | $\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$ | $jx(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J44007b | TrGJC | $\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HO}_2 + \text{HCOCO}_3\text{H}$ | J_ACETOL | Rickard and Pascoe (2009) |
| J44008 | TrGJC | $\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$ | $jx(\text{ip_MACR})$ | Sander et al. (2014) |
| J44009 | TrGJC | $\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$ | $jx(\text{ip_CH300H}) + 2.77 \cdot jx(\text{ip_HOCH}_2\text{CHO})$ | Taraborrelli (2016)* |
| J44010 | TrGJC | $\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$ | $2.77 \cdot jx(\text{ip_HOCH}_2\text{CHO})$ | see note* |
| J44011 | TrGJC | $\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$ | $jx(\text{ip_CH300H})$ | Taraborrelli (2016) |
| J44012 | TrGJC | $\text{LHMVKABOOH} + h\nu \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{CH}_3\text{C}(\text{O}) + .88 \text{HOCH}_2\text{CHO} + .12 \text{HCHO} + \text{OH}$ | $jx(\text{ip_CH300H}) + \text{J_ACETOL}$ | Taraborrelli (2016) |
| J44013 | TrGJC | $\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$ | $jx(\text{ip_HOCH}_2\text{CHO}) + \text{J_ACETOL}$ | Taraborrelli (2016) |
| J44014 | TrGJC | $\text{HO}_12\text{CO}_3\text{C}_4 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{HO}_2$ | J_ACETOL | Rickard and Pascoe (2009) |
| J44015 | TrGJC | $\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$ | $2.15 \cdot jx(\text{ip_MGLYOX})$ | see note* |
| J44016 | TrGC | $\text{HCOCCH}_3\text{CO} + h\nu \rightarrow .5 \text{OH} + .5 \text{CH}_3\text{CHO} + \text{CO} + .5 \text{CH}_3\text{CHCO} + .5 \text{CO}$ | J_KETENE | Taraborrelli (2016) |
| J44017a | TrGC | $\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{CH}_3\text{COCO}_2\text{H} + .1848 \text{H}_2\text{O}_2 + .2208 \text{MGLYOX} + .36 \text{OH} + .36 \text{CO} + .56 \text{CH}_3\text{C}(\text{O}) + .2 \text{CH}_3\text{CHO} + .2 \text{CO}_2 + .2 \text{HCHO} + .2 \text{HO}_2 + \text{CO}$ | $\text{J_KETENE} * 0.5$ | Taraborrelli (2016), Rickard and Pascoe (2009)* |
| J44017b | TrGC | $\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$ | $\text{J_KETENE} * 0.5$ | Taraborrelli (2016) |
| J44018a | TrGJC | $\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$ | $jx(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J44018b | TrGJC | $\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$ | $2.15 \cdot jx(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J44019 | TrGJC | $\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$ | $3.15 \cdot jx(\text{ip_MGLYOX})$ | Taraborrelli (2016) |
| J44020a | TrGJTerC | $\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$ | $jx(\text{ip_CH300H}) + \text{J_ACETOL}$ | Rickard and Pascoe (2009) |
| J44020b | TrGJTerC | $\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$ | $2.15 \cdot jx(\text{ip_MGLYOX})$ | Rickard and Pascoe (2009) |
| J44021 | TrGJTerC | $\text{C44OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$ | $jx(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J44022 | TrGJTerC | $\text{C413COOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$ | $jx(\text{ip_CH300H}) + jx(\text{ip_HOCH}_2\text{CHO}) + \text{J_ACETOL}$ | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|---|
| J44023a | TrGJTerC | $C4CODIAL + h\nu \rightarrow HCOCOCH_2O_2 + HO_2 + CO$ | $jx(ip_HOCH_2CHO)$ | Rickard and Pascoe (2009) |
| J44023b | TrGJTerC | $C4CODIAL + h\nu \rightarrow HCOCH_2CO_3 + HO_2 + CO$ | $jx(ip_MGLYOX)$ | Rickard and Pascoe (2009) |
| J44024 | TrGJTerC | $C312COCO_3H + h\nu \rightarrow HCOCOCH_2O_2 + CO_2 + OH$ | $jx(ip_CH300H)+jx(ip_MGLYOX)$ | Rickard and Pascoe (2009) |
| J44025 | TrGJCN | $LMEKNO_3 + h\nu \rightarrow .62 CH_3C(O) + .62 CH_3CHO + .38 HCHO$ $+ .38 CO_2 + .38 HOCH_2CH_2O_2 + NO_2$ | $jx(ip_MEKN03)$ | Barnes et al. (1993), Taraborrelli (2016)* |
| J44026 | TrGJCN | $MVKNO_3 + h\nu \rightarrow CH_3C(O) + HOCH_2CHO + NO_2$ | $jx(ip_MEKN03)$ | Barnes et al. (1993), Taraborrelli (2016)* |
| J44027 | TrGJCN | $MACRN + h\nu \rightarrow CH_3COCH_2OH + CO + HO_2 + NO_2$ | $(2.84*J_IC3H7N03+jx(ip_CH3CHO))$ $*(jx(ip_MEKN03)+1E-10)/(J_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)$ | Müller et al. (2014), Taraborrelli (2016)* |
| J44028 | TrGJCN | $TC4H9NO_3 + h\nu \rightarrow CH_3COCH_3 + CH_3 + NO_2$ | $2.84*J_IC3H7N03$ | Taraborrelli (2016) |
| J44029 | TrGJC | $TC_4H_9OOH + h\nu \rightarrow CH_3COCH_3 + CH_3 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44030 | TrGJCN | $IBUTOLBNO_3 + h\nu \rightarrow CH_3COCH_3 + HCHO + HO_2 + NO_2$ | $2.84*J_IC3H7N03$ | Taraborrelli (2016) |
| J44031 | TrGJC | $IBUTOLBOOH + h\nu \rightarrow CH_3COCH_3 + HCHO + HO_2 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44032 | TrGJC | $LBUT1ENOOH + h\nu \rightarrow C_2H_5CHO + HCHO + HO_2 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44033 | TrGJCN | $LBUT1ENNO_3 + h\nu \rightarrow C_2H_5CHO + HCHO + HO_2 + NO_2$ | $J_IC3H7N03$ | Taraborrelli (2016) |
| J44034 | TrGJC | $BUT2OLOOH + h\nu \rightarrow 2 CH_3CHO + HO_2 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44035 | TrGJCN | $BUT2OLNO_3 + h\nu \rightarrow 2 CH_3CHO + HO_2 + NO_2$ | $J_IC3H7N03$ | Taraborrelli (2016) |
| J44036 | TrGJC | $BUT2OLO + h\nu \rightarrow CH_3C(O) + HOCH_2CO$ | J_ACETOL | Taraborrelli (2016) |
| J44037a | TrGJC | $C_3H_7CHO + h\nu \rightarrow C_3H_7O_2 + CO + HO_2$ | $jx(ip_C3H7CHO2HCO)$ | Taraborrelli (2016) |
| J44037b | TrGJC | $C_3H_7CHO + h\nu \rightarrow C_2H_4 + CH_2CHOH$ | $jx(ip_C3H7CHO2VINY)$ | Taraborrelli (2016)* |
| J44038 | TrGJC | $IPRCHO + h\nu \rightarrow iC_3H_7O_2 + CO + HO_2$ | $jx(ip_IPRCHO2HCO)$ | Taraborrelli (2016) |
| J44039 | TrGJCN | $IC4H9NO_3 + h\nu \rightarrow IPRCHO + NO_2$ | $J_IC3H7N03$ | Taraborrelli (2016) |
| J44040 | TrGJC | $IC_4H_9OOH + h\nu \rightarrow IPRCHO + HO_2 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44041 | TrGJC | $PERIBUACID + h\nu \rightarrow iC_3H_7O_2 + CO_2 + OH$ | $jx(ip_CH300H)$ | Taraborrelli (2016) |
| J44042 | TrGJCN | $PIPn + h\nu \rightarrow .7 IPRCO_3 + .7 NO_2 + .3 iC_3H_7O_2 + .3 CO_2 +$ $.3 NO_3$ | $jx(ip_PAN)$ | Taraborrelli (2016), Sander et al. (2014), Sander et al. (2011) |
| J44043 | TrGJC | $HVMK + h\nu \rightarrow MGLYOX + CO + 2 OH$ | $jx(ip_PeDIONE24)$ | Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|--|--|---|
| J44044 | TrGJC | $\text{HMAC} + h\nu \rightarrow \text{HCOCCH}_3\text{CO} + 2 \text{OH}$ | $\text{jx}(\text{ip_PeDI0NE24})$ | Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)* |
| J44045a | TrGJC | $\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{HCO})$ | Rickard and Pascoe (2009) |
| J44045b | TrGJC | $\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$ | Andrews et al. (2012), Taraborrelli (2016) |
| J44046a | TrGJC | $\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{HCO}) * 2.$ | see note* |
| J44046b | TrGJC | $\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$ | $\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{ENOL}) * 2.$ | Andrews et al. (2012), Taraborrelli (2016) |
| J44200 | TrGJTerC | $\text{IBUTALOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{HO}_2 + \text{CO}$ | J_ACETOL | Rickard and Pascoe (2009) |
| J44201 | TrGJTerC | $\text{IPRHOCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009) |
| J44400a | TrGJAroC | $\text{MALDIALOOH} + h\nu \rightarrow \text{C}_3\text{O}_2\text{H}_3\text{CO} + \text{CO} + \text{OH} + \text{HO}_2$ | $\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2$ | Rickard and Pascoe (2009) |
| J44400b | TrGJAroC | $\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J44401 | TrGJAroC | $\text{BZFUOOH} + h\nu \rightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J44402 | TrGJAroC | $\text{HOCOC}_4\text{DIAL} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$ | Rickard and Pascoe (2009) |
| J44403 | TrGJAroCN | $\text{NBZFUOOH} + h\nu \rightarrow .5 \text{CO}_2\text{C}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J44404a | TrGJAroC | $\text{MALDALCO}_3\text{H} + h\nu \rightarrow \text{HCOC}_3\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_MACR})$ | Rickard and Pascoe (2009) |
| J44404b | TrGJAroC | $\text{MALDALCO}_3\text{H} + h\nu \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J44405 | TrGJAroC | $\text{EPXDLCO}_2\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO}_2 + \text{HO}_2$ | $2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$ | Rickard and Pascoe (2009) |
| J44406 | TrGJAroC | $\text{MALDIAL} + h\nu \rightarrow .4 \text{BZFUONE} + .6 \text{MALDIALCO}_3 + .6 \text{HO}_2$ | $\text{jx}(\text{ip_NO}_2) * 0.14$ | Rickard and Pascoe (2009) |
| J44407 | TrGJAroC | $\text{MALANHYOOH} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |
| J44408 | TrGJAroC | $\text{EPXDLCO}_3\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{OH} + \text{CO}_2$ | $\text{jx}(\text{ip_CH}_3\text{OOH}) + 2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$ | Rickard and Pascoe (2009) |
| J44409 | TrGJAroC | $\text{CO}_2\text{C}_4\text{DIAL} + h\nu \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{HO}_2 + \text{CO} + \text{CO}$ | $\text{jx}(\text{ip_MGLYOX}) * 2$ | Rickard and Pascoe (2009) |
| J44410 | TrGJAroC | $\text{MALDALCO}_2\text{H} + h\nu \rightarrow \text{HCOC}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_MACR})$ | Rickard and Pascoe (2009) |
| J44411 | TrGJAroC | $\text{EPXC}_4\text{DIAL} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO} + \text{HO}_2$ | $2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2$ | Rickard and Pascoe (2009) |
| J44412 | TrGJAroC | $\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$ | $\text{jx}(\text{ip_MGLYOX})$ | Rickard and Pascoe (2009) |
| J44414 | TrGJAroC | $\text{MECOACEOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH}_3\text{OOH})$ | Rickard and Pascoe (2009)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|--|--|--|
| J45002 | TrGJC | LISOPACOOH + hν → LISOPACO + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45003 | TrGJCN | LISOPACNO3 + hν → LISOPACO + NO ₂ | 0.59*J_IC3H7N03 | see note* |
| J45004 | TrGJC | ISOPBOOH + hν → MVK + HCHO + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45005 | TrGJCN | ISOPBNO3 + hν → MVK + HCHO + HO ₂ + NO ₂ | 2.84*J_IC3H7N03 | see note* |
| J45006 | TrGJC | ISOPDOOH + hν → MACR + HCHO + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45007 | TrGJCN | ISOPDNO3 + hν → MACR + HCHO + HO ₂ + NO ₂ | J_IC3H7N03 | see note* |
| J45008 | TrGJCN | NISOPOOH + hν → NC4CHO + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45009 | TrGJCN | NC4CHO + hν → LHC4ACCO3 + NO ₂ | (.59*J_IC3H7N03+jx(ip_MACR)) *(jx(ip_MEKN03)+1E-10)/(J_IC3H7N03+0.42*jx(ip_CHOH)+1E-10) | Müller et al. (2014), Taraborrelli (2016)* |
| J45010 | TrGJCN | LNISOOH + hν → NOA + OH + .5 HOCHCHO + .5 CO + .5 HO ₂ + .5 CO ₂ | jx(ip_CH300H) | Taraborrelli et al. (2009), Taraborrelli (2016) |
| J45011 | TrGJC | LHC4ACCHO + hν → .5 LHC4ACCO3 + .5 HO ₂ + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2 | jx(ip_MACR) | Taraborrelli (2016) |
| J45012 | TrGJC | LC578OOH + hν → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ + OH | jx(ip_CH300H)+ 2.77*jx(ip_HOCH2CHO) | Taraborrelli (2016) |
| J45013 | TrGJC | LHC4ACCO3H + hν → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO ₂ | J_HPALD | Taraborrelli (2016) |
| J45014 | TrGJCN | LC5PAN1719 + hν → .7 LHC4ACCO3 + .7 NO ₂ + .15 MACRO2 + .15 LHMVKABO2 + .3 CO ₂ + .3 NO ₃ | jx(ip_PAN) | Taraborrelli (2016) |
| J45015 | TrGJC | HCOC5 + hν → .65 CH ₃ + .65 CO + .65 HCHO + .35 OH + .35 CH ₃ COCH ₂ O ₂ + HOCH2CO | 0.5*jx(ip_MVK) | Taraborrelli (2016)* |
| J45016 | TrGJC | C59OOH + hν → CH ₃ COCH ₂ OH + HOCH2CO + OH | J_ACETOL+jx(ip_CH300H) | Taraborrelli (2016) |
| J45017 | TrGJTerC | C511OOH + hν → CH ₃ C(O) + HCOCH2CHO + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45018a | TrGJTerC | CO23C4CHO + hν → CH ₃ COCOCH ₂ O ₂ + HO ₂ + CO | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45018b | TrGJTerC | CO23C4CHO + hν → CH ₃ C(O) + HCOCH2CO3 | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45019 | TrGJTerC | CO23C4CO3H + hν → CH ₃ COCOCH ₂ O ₂ + CO ₂ + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45020 | TrGJTerC | C512OOH + hν → C513O2 + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45021 | TrGJTerC | CO13C4CHO + hν → CHOC3COO2 + CO + HO ₂ | jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J45022 | TrGJTerC | C513OOH + hν → GLYOX + HOC ₂ H ₄ CO ₃ + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45023 | TrGJTerC | C513CO + hν → HOC ₂ H ₄ CO ₃ + HO ₂ + CO + CO | jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45024 | TrGJTerC | C514OOH + hν → CO13C4CHO + HO ₂ + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |
| J45025 | TrGJTerCN | C514NO3 + hν → CO13C4CHO + HO ₂ + NO ₂ | J_IC3H7N03+jx(ip_HOCH2CHO)*2. | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|----------|--|--|--|
| J45026a | TrGJC | ZCODC23DBCOOH + $h\nu$ → OH + CO + HVMK + OH | J_HPALD*0.6*0.5 | Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026b | TrGJC | ZCODC23DBCOOH + $h\nu$ → OH + CO + CH ₃ C(O) + HOCH ₂ CHO | J_HPALD*0.6*0.5 | Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026c | TrGJC | ZCODC23DBCOOH + $h\nu$ → OH + CO + HMAc + OH | J_HPALD*0.4*0.5 | Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014) |
| J45026d | TrGJC | ZCODC23DBCOOH + $h\nu$ → OH + CO + CO + CH ₃ COCH ₂ OH + HO ₂ | J_HPALD*0.4*0.5 | Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014) |
| J45027 | TrGJC | ZCO3HC23DBCOD + $h\nu$ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO ₂ | J_HPALD | Taraborrelli (2016) |
| J45028a | TrGJC | C1OOHC2OOHC4OD + $h\nu$ → CH ₃ COCH ₂ O ₂ H + OH + 2 CO + HO ₂ | 2.77*JX(IP_HOCH2CHO) | Taraborrelli (2016) |
| J45028b | TrGJC | C1OOHC2OOHC4OD + $h\nu$ → .5 CH ₃ COCH ₂ O ₂ H + .5 HOCHCHO + .5 CO ₂ H3CHO + .5 HCHO + 1.5 OH | 2.*JX(IP_CH300H) | Taraborrelli (2016) |
| J45029 | TrGC | DB1OOH + $h\nu$ → DB1O2 + OH | JX(IP_CH300H) | Taraborrelli (2016) |
| J45030 | TrGC | DB2OOH + $h\nu$ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH | JX(ip_CH300H) | Taraborrelli (2016) |
| J45031a | TrGJC | C1ODC2OOHC4OD + $h\nu$ → MGLYOX + HOCHCHO + OH | JX(ip_CH300H) | Taraborrelli (2016) |
| J45031b | TrGJC | C1ODC2OOHC4OD + $h\nu$ → CO ₂ H3CHO + CO + HO ₂ + OH | 2.*2.77*JX(IP_HOCH2CHO) | Taraborrelli (2016) |
| J45032 | TrGJC | ZCODC23DBCOD + $h\nu$ → .5 CH ₃ COCHCO + .5 HCOCCH ₃ CO + CO + HO ₂ + OH | jx(ip_N02)*0.1*0.5 | Taraborrelli (2016)* |
| J45033 | TrGCN | DB1NO3 + $h\nu$ → DB1O2 + NO ₂ | J_IC3H7N03 | Taraborrelli (2016) |
| J45034 | TrGJTerC | CHOC3COOOH + $h\nu$ → CHOC3COO2 + CO ₂ + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL | Rickard and Pascoe (2009) |
| J45200a | TrGJTerC | LMBOABOOH + $h\nu$ → HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + OH | jx(ip_CH300H)*.67 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J45200b | TrGJTerC | LMBOABOOH + $h\nu$ → IBUTALOH + HCHO + HO ₂ + OH | jx(ip_CH300H)*.33 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J45201 | TrGJTerC | MBOACO + $h\nu$ → HCHO + HO ₂ + IPRHOCO3 | J_ACETOL | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|---|--|--|
| J45202 | TrGJTerC | MBOCOCO + hν → CO + HO ₂ + IPRHOCO3 | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45203a | TrGJTerCN | LNMBOABOOH + hν → NO ₃ CH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + OH | jx(ip_CH300H)*.65 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J45203b | TrGJTerCN | LNMBOABOOH + hν → IBUTALOH + HCHO + NO ₂ + OH | jx(ip_CH300H)*.35 | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J45204 | TrGJTerCN | NC4OHCO3H + hν → IBUTALOH + CO ₂ + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45400 | TrGJAroC | C54CO + hν → HO ₂ + CO + CO + CO + CH ₃ C(O) | jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)*2 | Rickard and Pascoe (2009) |
| J45401 | TrGJAroC | C5134CO2OH + hν → CH ₃ COCOCHO + HO ₂ + CO + HO ₂ | jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J45402 | TrGJAroC | C5DIALOOH + hν → MALDIAL + CO + HO ₂ + OH | jx(ip_CH300H)+jx(ip_MACR) | Rickard and Pascoe (2009)* |
| J45406 | TrGJAroC | C5CO14OH + hν → CH ₃ C(O) + HCOCO ₂ H + HO ₂ + CO | jx(ip_MVK) | Rickard and Pascoe (2009) |
| J45407 | TrGJAroC | C5DICARB + hν → .6 C5CO14O2 + .6 HO ₂ + .4 TLFUONE | jx(ip_NO2)*0.2 | Rickard and Pascoe (2009)* |
| J45408 | TrGJAroC | MC3ODBCO2H + hν → CH ₃ COCO ₂ H + HO ₂ + CO + HO ₂ + CO | jx(ip_MACR) | Rickard and Pascoe (2009) |
| J45409 | TrGJAroC | ACCOMMECHO + hν → MECOACETO2 + HO ₂ + CO | jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J45410 | TrGJAroC | MMALNHOOH + hν → CO2H3CO3 + CO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J45411 | TrGJAroC | C5DICAROOH + hν → MGLYOX + GLYOX + HO ₂ + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL | Rickard and Pascoe (2009)* |
| J45412 | TrGJAroCN | NTLFUOOH + hν → ACCOMECHO + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J45414 | TrGJAroC | C5CO14OOH + hν → .83 MALANHY + .83 CH ₃ + .17 MGLYOX + .17 HO ₂ + .17 CO + .17 CO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J45415 | TrGJAroC | TLFUOOH + hν → ACCOMECHO + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J45417 | TrGJAroC | ACCOMECO3H + hν → MECOACETO2 + CO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J45418 | TrGJAroC | C5DIALCO + hν → MALDIALCO3 + CO + HO ₂ | jx(ip_MGLYOX)+jx(ip_MACR) | Rickard and Pascoe (2009) |
| J46200 | TrGJTerCN | C614NO3 + hν → CO23C4CHO + HCHO + HO ₂ + NO ₂ | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46201 | TrGJTerC | C614OOH + hν → CO23C4CHO + HCHO + HO ₂ + OH | jx(ip_CH300H)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J46202 | TrGJTerC | CO235C5CHO + hν → CO23C4CO3 + CO + HO ₂ | jx(ip_MGLYOX) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|--------|-----------|--|--|----------------------------|
| J46203 | TrGJTerC | $\text{CO235C6OOH} + h\nu \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$ | $\text{jx}(\text{ip_CH300H}) + 2.15 * \text{jx}(\text{ip_MGLYOX})$ | Rickard and Pascoe (2009) |
| J46400 | TrGJAroC | $\text{PHENO0H} + h\nu \rightarrow .71 \text{ MALDALCO2H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46401 | TrGJAroC | $\text{C6CO4DB} + h\nu \rightarrow \text{C4CO2DBC03} + \text{HO}_2 + \text{CO}$ | $\text{jx}(\text{ip_MGLYOX}) * 2$ | Rickard and Pascoe (2009) |
| J46402 | TrGJAroC | $\text{C5CO2DCO3H} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_MGLYOX})$ | Rickard and Pascoe (2009) |
| J46403 | TrGJAroCN | $\text{NDNPHE00H} + h\nu \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46404 | TrGJAroCN | $\text{BZBIPERNO3} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{NO}_2$ | J_IC3H7N03 | Rickard and Pascoe (2009)* |
| J46405 | TrGJAroCN | $\text{HOC6H4NO2} + h\nu \rightarrow \text{HONO} + \text{CPDKETENE}$ | $\text{jx}(\text{ip_HOC6H4N02})$ | Chen et al. (2011)* |
| J46406 | TrGJAroC | $\text{CPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{ HO}_2 + \text{MALDIAL}$ | J_KETENE | see note* |
| J46407 | TrGJAroC | $\text{C5COOHCO3H} + h\nu \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J46408 | TrGJAroC | $\text{BZEPOXMUC} + h\nu \rightarrow .5 \text{ C5DIALO2} + 1.5 \text{ HO}_2 + 1.5 \text{ CO} + .5 \text{ MALDIAL}$ | $4.E3 * \text{jx}(\text{ip_MVK}) * 0.1$ | Rickard and Pascoe (2009) |
| J46409 | TrGJAroCN | $\text{NPHEN1OOH} + h\nu \rightarrow \text{NPHEN1O} + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J46410 | TrGJAroC | $\text{BZEMUCCO} + h\nu \rightarrow \text{HCOCOHC03} + \text{C3DIALO2}$ | $\text{jx}(\text{ip_HOCH2CH0}) * 2 + \text{J_ACETOL}$ | Rickard and Pascoe (2009) |
| J46411 | TrGJAroC | $\text{BZEMUCCO2H} + h\nu \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{HO}_2$ | $\text{jx}(\text{ip_MACR})$ | Rickard and Pascoe (2009) |
| J46412 | TrGJAroCN | $\text{NNCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46413 | TrGJAroC | $\text{C615CO2OOH} + h\nu \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_MVK}) + \text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J46414 | TrGJAroCN | $\text{NPHE00H} + h\nu \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{OH} + \text{NO}_2$ | $\text{J_IC3H7N03} + \text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J46415 | TrGJAroCN | $\text{NCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46416 | TrGJAroC | $\text{PBZQOOH} + h\nu \rightarrow \text{C5CO2OHCO3} + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46417 | TrGJAroC | $\text{BZOBIPEROH} + h\nu \rightarrow \text{MALDIALCO3} + \text{GLYOX} + \text{HO}_2$ | J_ACETOL | Rickard and Pascoe (2009) |
| J46418 | TrGJAroC | $\text{BZBIPEROOH} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46419 | TrGJAroCN | $\text{NBZQOOH} + h\nu \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |
| J46420 | TrGJAroC | $\text{CATEC1OOH} + h\nu \rightarrow \text{CATEC1O} + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009) |
| J46421 | TrGJAroC | $\text{C6125CO} + h\nu \rightarrow \text{C5CO14O2} + \text{CO} + \text{HO}_2$ | $\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_MVK})$ | Rickard and Pascoe (2009) |
| J46422 | TrGJAroCN | $\text{DNPHENO0H} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$ | $\text{jx}(\text{ip_CH300H})$ | Rickard and Pascoe (2009)* |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|---|----------------------------------|--------------------------------|
| J46423 | TrGJAroC | BZEMUCCO3H + hν → C5DIALO2 + CO ₂ + OH | jx(ip_CH300H)+jx(ip_MACR) | Rickard and Pascoe (2009) |
| J46424 | TrGJAroC | C6H5OOH + hν → C6H5O + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J46425 | TrGJAroC | BZEMUCOOH + hν → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO)*2 | Rickard and Pascoe (2009)* |
| J46427 | TrGJAroCN | BZEMUCNO3 + hν → EPXC4DIAL + NO ₂ + GLYOX + HO ₂ | 2.77*jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J46428 | TrGJAroCN | DNPHEN + hν → HONO + NCPDKETENE | jx(ip_HOC6H4N02) | Taraborrelli (2016) |
| J46429 | TrGJAroCN | NCPDKETENE + hν → CO ₂ + CO + 2 HO ₂ + NC4DCO2H | J_KETENE | see note* |
| J47200 | TrGJTerC | CO235C6CHO + hν → CHOC3COCO3 + CH ₃ C(O) | 2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J47201 | TrGJTerC | C235C6CO3H + hν → CO235C6O2 + CO ₂ + OH | jx(ip_CH300H)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J47202 | TrGJTerC | C716OOH + hν → CO13C4CHO + CH ₃ C(O) + OH | jx(ip_CH300H)+jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J47203 | TrGJTerC | C721OOH + hν → C722O2 + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47204 | TrGJTerC | C722OOH + hν → CH ₃ COCH ₃ + C44O2 + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47400 | TrGJAroC | TLEPOXMUC + hν → .5 C615CO2O2 + HO ₂ + CO + .5 EPXC4DIAL + .5 CH ₃ C(O) | 4.E3*jx(ip_MVK)*0.1 | Rickard and Pascoe (2009) |
| J47401 | TrGJAroC | C6H5CH2OOH + hν → BENZAL + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47402 | TrGJAroCN | C6H5CH2NO3 + hν → BENZAL + HO ₂ + NO ₂ | 0.59*J_IC3H7N03 | Rickard and Pascoe (2009)* |
| J47403 | TrGJAroC | BENZAL + hν → HO ₂ + CO + C6H5O2 | jx(ip_BENZAL) | T. J. Wallington et al. (2014) |
| J47404 | TrGJAroC | TLBIPEROOH + hν → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47405 | TrGJAroCN | TLBIPERNO3 + hν → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO ₂ | J_IC3H7N03 | Rickard and Pascoe (2009)* |
| J47406 | TrGJAroC | TLOBIPEROH + hν → C5CO14O2 + GLYOX + HO ₂ | J_ACETOL | Rickard and Pascoe (2009) |
| J47407 | TrGJAroC | CRESOOH + hν → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47408a | TrGJAroCN | NCRESOOH + hν → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH + NO ₂ | J_IC3H7N03 | Rickard and Pascoe (2009)* |
| J47408b | TrGJAroCN | NCRESOOH + hν → C5CO14OH + GLYOX + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47409 | TrGJAroCN | TOL1OHNO2 + hν → HONO + MCPDKETENE | jx(ip_HOPh3Me2N02) | see note* |
| J47410 | TrGJAroC | TLEMUCCO2H + hν → C615CO2O2 + CO ₂ + HO ₂ | jx(ip_MACR) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|--------|-----------|---|---|----------------------------|
| J47411 | TrGJAroC | TLEMUCCO3H + hν → C615CO2O2 + CO ₂ + OH | jx(ip_CH300H)+jx(ip_MACR) | Rickard and Pascoe (2009) |
| J47412 | TrGJAroC | TLEMUCOOH + hν → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH | jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)+J_ACETOL | Rickard and Pascoe (2009)* |
| J47413 | TrGJAroCN | TLEMUCNO3 + hν → EPXC4DIAL + NO ₂ + CH ₃ C(O) + CO + HO ₂ | 2.77*jx(ip_HOCH2CHO)+J_ACETOL | Rickard and Pascoe (2009) |
| J47414 | TrGJAroC | TLEMUCCO + hν → CH ₃ C(O) + EPXC4DIAL + CO + HO ₂ | 2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX) | Rickard and Pascoe (2009) |
| J47415 | TrGJAroC | C6H5CO3H + hν → C6H5O2 + CO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47416 | TrGJAroC | OXYL1OOH + hν → TOL1O + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47417 | TrGJAroCN | MNCATECH + hν → HONO + MCPDKETENE | jx(ip_HOPh3Me2N02) | see note* |
| J47418 | TrGJAroC | MCPDKETENE + hν → CO ₂ + CO + 2 HO ₂ + ZCODC23DBCOD | J_KETENE | see note* |
| J47419 | TrGJAroCN | DNCREs + hν → HONO + MNCPDKETENE | jx(ip_HOPh3Me2N02) | see note* |
| J47420 | TrGJAroCN | MNCPDKETENE + hν → CO ₂ + CO + 2 HO ₂ + NC4MDCO2HN | J_KETENE | see note* |
| J47421 | TrGJAroC | MCATEC1OOH + hν → MCATEC1O + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47422 | TrGJAroCN | NPTLQOOH + hν → C7CO4DB + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47423 | TrGJAroC | PTLQOOH + hν → C6CO2OHCO3 + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47424 | TrGJAroCN | NCRES1OOH + hν → NCRES1O + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J47425 | TrGJAroCN | MNNCATCOOH + hν → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47426 | TrGJAroCN | MNCATECOOH + hν → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47427 | TrGJAroC | C7CO4DB + hν → C5CO2DBC03 + HO ₂ + CO | jx(ip_MGLYOX)*2 | Rickard and Pascoe (2009) |
| J47428 | TrGJAroCN | NDNCRESOOH + hν → NC4MDCO2HN + HNO ₃ + CO + CO + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47429 | TrGJAroCN | DNCRESOOH + hν → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009)* |
| J47430 | TrGJAroC | C6COOHCO3H + hν → C5134CO2OH + HO ₂ + CO + CO ₂ + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J48200 | TrGJTerC | C86OOH + hν → C511O2 + CH ₃ COCH ₃ + OH | jx(ip_CH300H)+ jx(ip_HOCH2CHO) | Rickard and Pascoe (2009) |
| J48201 | TrGJTerC | C812OOH + hν → C813O2 + OH | jx(ip_CH300H) | Rickard and Pascoe (2009) |
| J48202 | TrGJTerC | C813OOH + hν → CH ₃ COCH ₃ + C512O2 + OH | jx(ip_CH300H)+jx(ip_MGLYOX) | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|---------|-----------|---|--|--|
| J48203 | TrGJTerC | $C721CHO + h\nu \rightarrow C721O2 + CO + HO_2$ | $jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J48204 | TrGJTerC | $C721CO3H + h\nu \rightarrow C721O2 + CO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J48205 | TrGJTerC | $C8BCOOH + h\nu \rightarrow C89O2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J48206 | TrGJTerC | $C89OOH + h\nu \rightarrow C810O2 + OH$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J48207 | TrGJTerCN | $C89NO3 + h\nu \rightarrow C810O2 + NO_2$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J48208 | TrGJTerC | $C810OOH + h\nu \rightarrow CH_3COCH_3 + C514O2 + OH$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J48209 | TrGJTerCN | $C810NO3 + h\nu \rightarrow CH_3COCH_3 + C514O2 + NO_2$ | $2.84*J_IC3H7N03+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J48210 | TrGJTerCN | $C8BCNO3 + h\nu \rightarrow C89O2 + NO_2$ | $J_IC3H7N03$ | Rickard and Pascoe (2009) |
| J48211 | TrGJTerC | $C85OOH + h\nu \rightarrow C86O2 + OH$ | $jx(ip_CH300H)+J_ACETOL$ | Rickard and Pascoe (2009) |
| J48400 | TrGJAroC | $STYRENOOH + h\nu \rightarrow HO_2 + HCHO + BENZAL + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009)* |
| J49200 | TrGJTerC | $C96OOH + h\nu \rightarrow C97O2 + OH$ | $jx(ip_CH300H)+J_ACETOL$ | Rickard and Pascoe (2009) |
| J49201 | TrGJTerC | $C97OOH + h\nu \rightarrow C98O2 + OH$ | $jx(ip_CH300H)+J_ACETOL$ | Rickard and Pascoe (2009) |
| J49202 | TrGJTerC | $C98OOH + h\nu \rightarrow C614O2 + CH_3COCH_3 + OH$ | $(jx(ip_CH300H)+2.15*jx(ip_MGLYOX))$ | Rickard and Pascoe (2009) |
| J49203a | TrGJTerC | $NORPINAL + h\nu \rightarrow C85O2 + CO + HO_2$ | $jx(ip_PINAL2HCO)$ | Rickard and Pascoe (2009), Taraborrelli (2016) |
| J49203b | TrGJTerC | $NORPINAL + h\nu \rightarrow NORPINENOL$ | $jx(ip_PINAL2ENOL)$ | Taraborrelli (2016), Andrews et al. (2012) |
| J49204 | TrGJTerC | $C85CO3H + h\nu \rightarrow C85O2 + CO_2 + OH$ | $jx(ip_CH300H)+J_ACETOL$ | Rickard and Pascoe (2009) |
| J49205 | TrGJTerC | $C89CO2H + h\nu \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2 + HO_2$ | $jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J49206 | TrGJTerC | $C89CO3H + h\nu \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2 + OH$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J49207 | TrGJTerC | $C811CO3H + h\nu \rightarrow C811O2 + CO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J49208 | TrGJTerC | $NOPINDOOH + h\nu \rightarrow C89CO3 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J40200 | TrGJTerC | $LAPINABOOH + h\nu \rightarrow PINAL + HO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J40201 | TrGJTerC | $MENTHEN6ONE + h\nu \rightarrow RO6R1O2 + OH$ | $jx(ip_CH300H)$ | Vereecken et al. (2007) |
| J40202 | TrGJTerC | $2OHMENTHEN6ONE + h\nu \rightarrow 10 LCARBON + OH$ | $jx(ip_CH300H)$ | Vereecken et al. (2007) |
| J40203a | TrGJTerC | $PINAL + h\nu \rightarrow C96O2 + CO + HO_2$ | $jx(ip_PINAL2HCO)$ | Rickard and Pascoe (2009) |
| J40203b | TrGJTerC | $PINAL + h\nu \rightarrow PINEOL$ | $jx(ip_PINAL2ENOL)$ | Taraborrelli (2016), Andrews et al. (2012)* |
| J40204 | TrGJTerC | $PERPINONIC + h\nu \rightarrow C96O2 + CO_2 + OH$ | $jx(ip_CH300H)+J_ACETOL$ | Rickard and Pascoe (2009) |
| J40205 | TrGJTerC | $PINALOOH + h\nu \rightarrow C106O2 + OH$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J40206 | TrGJTerCN | $PINALNO3 + h\nu \rightarrow C106O2 + NO_2$ | $J_IC3H7N03+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J40207 | TrGJTerC | $C106OOH + h\nu \rightarrow C716O2 + CH_3COCH_3 + OH$ | $jx(ip_CH300H)+jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |

Table 2: Photolysis reactions (... continued)

| # | labels | reaction | rate coefficient | reference |
|--------|-----------|--|---------------------------------------|---------------------------|
| J40208 | TrGJTerCN | $C106NO_3 + h\nu \rightarrow C716O_2 + CH_3COCH_3 + NO_2$ | $J_IC3H7N03 + jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J40209 | TrGJTerC | $C109OOH + h\nu \rightarrow C89CO_3 + HCHO + OH$ | $jx(ip_CH300H) + jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J40210 | TrGJTerC | $C109CO + h\nu \rightarrow C89CO_3 + CO + HO_2$ | $jx(ip_MGLYOX) + jx(ip_HOCH2CHO)$ | Rickard and Pascoe (2009) |
| J40211 | TrGJTerCN | $LNAPINABOOH + h\nu \rightarrow PINAL + NO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J40212 | TrGJTerC | $BPINAOOH + h\nu \rightarrow NOPINONE + HCHO + HO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J40213 | TrGJTerCN | $LNBPINABOOH + h\nu \rightarrow NOPINONE + HCHO + NO_2 + OH$ | $jx(ip_CH300H)$ | Rickard and Pascoe (2009) |
| J40214 | TrGJTerCN | $ROO6R1NO_3 + h\nu \rightarrow ROO6R3O_2 + CH_3COCH_3 + NO_2$ | $2.84 * J_IC3H7N03 + jx(ip_CH300H)$ | Taraborrelli (2016) |
| J40215 | TrGJTerCN | $RO6R1NO_3 + h\nu \rightarrow 9 \text{ L CARBON} + HCHO + HO_2 + NO_2$ | $2.84 * J_IC3H7N03$ | Taraborrelli (2016) |

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:

$J(11) \rightarrow jx(ip_COH2)$
 $J(12) \rightarrow jx(ip_CHOH)$
 $J(15) \rightarrow jx(ip_HOCH2CHO)$
 $J(18) \rightarrow jx(ip_MACR)$
 $J(22) \rightarrow jx(ip_ACETOL)$
 $J(23)+J(24) \rightarrow jx(ip_MVK)$
 $J(31)+J(32)+J(33) \rightarrow jx(ip_GLYOX)$
 $J(34) \rightarrow jx(ip_MGLYOX)$
 $J(41) \rightarrow jx(ip_CH300H)$
 $J(53) \rightarrow J(iC_3H_7ONO_2)$
 $J(54) \rightarrow J(iC_3H_7ONO_2)$
 $J(55) \rightarrow J(iC_3H_7ONO_2)$
 $J(56)+J(57) \rightarrow jx(ip_NOA)$

Specific notes

J41006: product distribution as for HNO₄

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(NO₃CH₂CHO) is the same as J(PAN).

J42021: In analogy to what is assumed for CH₃O₂NO₂ 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 $J(C_3H_7ONO_2) = 0.59 \times J(iC_3H_7ONO_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J43025a: Photolysis frequencies very similar to the ones of CH₃CHO.

J43025b: Photolysis frequencies very similar to the ones of CH₃CHO.

J43400: KDEC C3DIALO \rightarrow 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(iC₃H₇ONO₂).

J44005b: It is assumed that J(LC4H9NO₃) is the same as J(iC₃H₇ONO₂).

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(HOCH₂CHO), 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(HOCH₂CHO), 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 Criegee Intermediate is assumed to solely react with water.

J44025: J values only for the secondary nitrate.

J44026: Like for LMEKNO3 photolysis

J44027: $2.84 \times \text{J}_{\text{IC3H7NO3}}$ 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 photo- tautomerization.

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: $\text{KDEC MALDIALO} \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2$

J44401: $\text{KDEC BZFUO} \rightarrow \text{CO14O3CHO} + \text{HO}_2$

J44403: $\text{KDEC NBZFUO} \rightarrow .5 \text{CO14O3CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2$

J44404b: $\text{KDEC MALDIALCO}_2 \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO}$

J44407: $\text{KDEC MALANHYO} \rightarrow \text{HCOCO2HCO}_3$

J44414: $\text{KDEC MECOACETO} \rightarrow \text{CH}_3\text{CO}_3 + \text{HCHO}$

J45003: It is assumed that $\text{J}(\text{LISOPACNO}_3) = 0.59 \times \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that $\text{J}(\text{ISOPBNO}_3) = 2.84 \times \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that $\text{J}(\text{ISOPDNO}_3)$ is the same as $\text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J45009: $0.59 \times \text{J}_{\text{IC3H7NO3}}$ 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 $\text{J}(\text{HCOC5})$ is half as large as $\text{J}(\text{MVK})$. With exception of HOCH_2CO the products of MACO_2 decomposition without CO_2 .

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

J45402: $\text{KDEC C5DIALO} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2$

J45407: $\text{KDEC TLFUONE} \rightarrow .6 \text{C5CO14O}_2 + .6 \text{HO}_2 + .4 \text{TLFUONE}$

J45410: $\text{KDEC MMALANHYO} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$

J45411: $\text{KDEC C5DICARBO} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2$

J45412: $\text{KDEC NTLFUO} \rightarrow \text{ACCOMECHEO} + \text{NO}_2$

J45414: $\text{KDEC C5CO14CO}_2 \rightarrow .83 \text{MALANHY} + .83 \text{CH}_3 + .17 \text{MGLYOX} + .17 \text{HO}_2 + .17 \text{CO} + .17 \text{CO}_2$

J45415: $\text{KDEC TLFUO} \rightarrow \text{ACCOMECHEO} + \text{HO}_2$

J46400: $\text{KDEC PHENO} \rightarrow .71 \text{MALDALCO}_2\text{H} + .71 \text{GLYOX} + .29 \text{PBZQONE} + \text{HO}_2$

J46403: $\text{KDEC NDNPHENO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2$

J46404: $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{BZFUONE} + .5 \text{BZFUONE}$

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: $\text{KDEC NNCATECO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$

J46415: $\text{KDEC NCATECO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{HO}_2$

J46416: $\text{KDEC PBZQO} \rightarrow \text{C5CO}_2\text{OHCO}_3$

J46418: $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{BZFUONE} + .5 \text{BZFUONE}$

J46419: $\text{KDEC NBZQO} \rightarrow \text{C6CO}_4\text{DB} + \text{NO}_2$

J46422: $\text{KDEC DNPHEO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$

J46425: $\text{KDEC BZEMUCO} \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C3}_2\text{OH13CO}$

J46429: new channel

J47401: $\text{KROPRIM}^*\text{O}_2$ fast reaction $\text{C}_6\text{H}_5\text{CH}_2\text{O} = \text{BENZAL} + \text{HO}_2$

J47402: $\text{KROPRIM}^*\text{O}_2$ fast reaction $\text{C}_6\text{H}_5\text{CH}_2\text{O} = \text{BENZAL} + \text{HO}_2$

J47404: $\text{KDEC TLBIPERO} \rightarrow .6 \text{GLYOX} + .4 \text{MGLYOX} + \text{HO}_2 + .2 \text{ZCODC23DBCOD} + .2 \text{C5DICARB} + .2 \text{TLFUONE} + .2 \text{BZFUONE} + .2 \text{MALDIAL}$

J47405: $\text{KDEC TLBIPERO} \rightarrow .6 \text{GLYOX} + .4 \text{MGLYOX} + \text{HO}_2 + .2 \text{ZCODC23DBCOD} + .2 \text{C5DICARB} + .2 \text{TLFUONE} + .2 \text{BZFUONE} + .2 \text{MALDIAL}$

J47407: $\text{KDEC CRESO} \rightarrow .68 \text{C5CO14OH} + .68 \text{GLYOX} + \text{HO}_2 + .32 \text{PTLQONE}$

| | | |
|--|--|---|
| J47408a: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE | J47418: new channel | J47428: KDEC NDNCRESO \rightarrow NC4MDCO ₂ H + HNO ₃ + CO + CO + NO ₂ |
| J47408b: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO ₂ | J47419: Using J for 3-methyl-2-nitrophenol. | J47429: KDEC DNCRESO \rightarrow NC4MDCO ₂ H + HCOCO ₂ H + NO ₂ |
| J47409: Using J for 3-methyl-2-nitrophenol. | J47420: new channel | J48400: KDEC STYRENO \rightarrow HO ₂ + HCHO + BENZAL |
| J47412: KDEC TLEMUCO \rightarrow .5 C3DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ | J47422: KDEC NPTLQO \rightarrow C7CO4DB + NO ₂ | J40203b: Substituted vinyl alcohol in analogy to CH ₃ CHO photolysis. |
| J47417: Using J for 3-methyl-2-nitrophenol. | J47423: KDEC PTLQO \rightarrow C6CO ₂ OHCO ₃ | |
| | J47425: KDEC MNNCATECO \rightarrow NC4MDCO ₂ H + HCOCO ₂ H + NO ₂ | |
| | J47426: KDEC MNCATECO \rightarrow NC4MDCO ₂ H + HCOCO ₂ H + HO ₂ | |

Table 3: Henry's law coefficients

| substance | k_H^\ominus M/atm | $-\Delta_{\text{soln}}H/R$ K | reference |
|--|--------------------------------------|---------------------------------|---------------------------------|
| O ₂ | 1.3×10^{-3} | 1500. | Wilhelm et al. (1977) |
| O ₃ | 1.2×10^{-2} | 2560. | Chameides (1984) |
| OH | 3.0×10^1 | 4300. | Hanson et al. (1992) |
| HO ₂ | 3.9×10^3 | 5900. | Hanson et al. (1992) |
| H ₂ O ₂ | $1. \times 10^5$ | 6338. | Lind and Kok (1994) |
| H ₂ O | BIG | 0. | see note |
| NH ₃ | 58. | 4085. | Chameides (1984) |
| NO | 1.9×10^{-3} | 1480. | Schwartz and White (1981) |
| NO ₂ | 7.0×10^{-3} | 2500. | Lee and Schwartz (1981)* |
| NO ₃ | 2. | 2000. | Thomas et al. (1993) |
| N ₂ O ₅ | BIG | 0. | see note |
| HONO | 4.9×10^1 | 4780. | Schwartz and White (1981) |
| HNO ₃ | $2.45 \times 10^6 / 1.5 \times 10^1$ | 8694. | Brimblecombe and Clegg (1989)* |
| HNO ₄ | 1.2×10^4 | 6900. | Régimbal and Mozurkewich (1997) |
| CH ₃ OH | 2.20×10^2 | 5200. | Snider and Dawson (1985) |
| CH ₃ O ₂ | 6. | 5600. | Jacob (1986)* |
| CH ₃ OOH | 3.0×10^2 | 5322. | Lind and Kok (1994) |
| CO ₂ | 3.1×10^{-2} | 2423. | Chameides (1984) |
| HCHO | 7.0×10^3 | 6425. | Chameides (1984) |
| HCOOH | 3.7×10^3 | 5700. | Chameides (1984) |
| CH ₃ COOH | 4.1×10^3 | 6200. | Sander et al. (2006) |
| PAN | 2.8 | 5730. | Sander et al. (2006) |
| C ₂ H ₅ O ₂ | 6. | 5600. | see note |
| CH ₃ CHO | 1.29×10^1 | 5890. | Sander et al. (2006) |
| GLYOX | 4.19×10^5 | 7481. | Sander et al. (2011) |
| HOCH ₂ CO ₂ H | 2.83×10^4 | 4029. | Ip et al. (2009) |
| HOCH ₂ CHO | 4.10×10^4 | 4600. | Betterton and Hoffmann (1988) |
| CH ₃ COCH ₃ | 28.1 | 5050. | Sander et al. (2006) |
| MGLYOX | 3.70×10^3 | 7500. | Betterton and Hoffmann (1988) |
| SO ₂ | 1.2 | 3120. | Chameides (1984) |
| H ₂ SO ₄ | $1. \times 10^{11}$ | 0. | see note |
| CH ₃ SO ₃ H | BIG | 0. | see note |
| DMS | 5.4×10^{-1} | 3500. | Staudinger and Roberts (2001) |

Table 3: Henry's law coefficients (... continued)

| substance | $\frac{k_H^\ominus}{\text{M/atm}}$ | $\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$ | reference |
|-----------|------------------------------------|---|-------------------------|
| DMSO | $5. \times 10^4$ | 6425. | De Bruyn et al. (1994)* |

General notes

The value "BIG" corresponds to virtually infinite solubility which is represented in the model using a very large but arbitrary number.

The temperature dependence of the Henry constants is:

$$K_H = K_H^\ominus \times \exp\left(\frac{-\Delta_{\text{soln}}H}{R} \left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right)$$

where $\Delta_{\text{soln}}H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314 \text{ J}/(\text{mol K})$.

Specific notes

NO₂: The temperature dependence is from Chameides (1984).

HNO₃: Calculated using the acidity constant from Davis and de Bruin (1964).

CH₃O₂: This value was estimated by Jacob (1986).

C₂H₅O₂: Assumed to be the same as $K_H(\text{CH}_3\text{O}_2)$.

H₂SO₄: To account for the very high Henry's law coefficient of H₂SO₄, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

| substance | α^\ominus | $\frac{-\Delta_{\text{obs}}H/R}{K}$ | reference |
|--|-----------------------|-------------------------------------|-------------------------------|
| O ₂ | 0.01 | 2000. | see note |
| O ₃ | 0.002 | (default) | DeMore et al. (1997)* |
| OH | 0.01 | (default) | Takami et al. (1998)* |
| HO ₂ | 0.5 | (default) | Thornton and Abbatt (2005) |
| H ₂ O ₂ | 0.077 | 3127. | Worsnop et al. (1989) |
| H ₂ O | 0.0 | (default) | see note |
| NH ₃ | 0.06 | (default) | DeMore et al. (1997)* |
| NO | 5.0×10^{-5} | (default) | Saastad et al. (1993)* |
| NO ₂ | 0.0015 | (default) | Ponche et al. (1993)* |
| NO ₃ | 0.04 | (default) | Rudich et al. (1996)* |
| N ₂ O ₅ | (default) | (default) | DeMore et al. (1997)* |
| HONO | 0.04 | (default) | DeMore et al. (1997)* |
| HNO ₃ | 0.5 | (default) | Abbatt and Waschewsky (1998)* |
| HNO ₄ | (default) | (default) | DeMore et al. (1997)* |
| CH ₃ OH | (default) | (default) | see note |
| CH ₃ O ₂ | 0.01 | 2000. | see note |
| CH ₃ OOH | 0.0046 | 3273. | Magi et al. (1997) |
| CO ₂ | 0.01 | 2000. | see note |
| HCHO | 0.04 | (default) | DeMore et al. (1997)* |
| HCOOH | 0.014 | 3978. | DeMore et al. (1997) |
| CH ₃ COOH | 2.0×10^{-2} | 4079. | Davidovits et al. (1995) |
| PAN | (default) | (default) | see note |
| C ₂ H ₅ O ₂ | (default) | (default) | see note |
| CH ₃ CHO | 3.0×10^{-2} | (default) | see note |
| GLYOX | (default) | (default) | see note |
| HOCH ₂ CO ₂ H | (default) | (default) | see note |
| HOCH ₂ CHO | (default) | (default) | see note |
| CH ₃ COCH ₃ | 3.72×10^{-3} | 6395. | Davidovits et al. (1995) |
| MGLYOX | (default) | (default) | see note |
| SO ₂ | 0.11 | (default) | DeMore et al. (1997) |
| H ₂ SO ₄ | 0.65 | (default) | Pöschl et al. (1998)* |
| CH ₃ SO ₃ H | 0.076 | 1762. | De Bruyn et al. (1994) |
| DMS | (default) | (default) | see note |
| DMSO | 0.048 | 2578. | De Bruyn et al. (1994) |

General notes

If no data are available, the following default values are used:

$$\alpha^{\ominus} = 0.1$$

$$-\Delta_{\text{obs}}H/R = 0 \text{ K}$$

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\begin{aligned} \frac{\alpha}{1-\alpha} &= \exp\left(\frac{-\Delta_{\text{obs}}G}{RT}\right) \\ &= \exp\left(\frac{-\Delta_{\text{obs}}H}{RT} + \frac{\Delta_{\text{obs}}S}{R}\right) \end{aligned}$$

where $\Delta_{\text{obs}}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\text{obs}}H$ and $\Delta_{\text{obs}}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\text{obs}}H}{R} \times \frac{1}{T} + \frac{-\Delta_{\text{obs}}S}{R}$$

and further:

$$d \ln\left(\frac{\alpha}{1-\alpha}\right) / d\left(\frac{1}{T}\right) = \frac{-\Delta_{\text{obs}}H}{R}$$

Specific notes

O₂: Estimate.

O₃: Value measured at 292 K.

OH: Value measured at 293 K.

NH₃: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO₂: Value measured at 298 K.

NO₃: Value is a lower limit, measured at 273 K.

N₂O₅: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO₃: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO₄: Value measured at 200 K for water ice.

CH₃O₂: Estimate.

CO₂: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

C₂H₅O₂: Estimate.

CH₃CHO: Using the same estimate as in the CAPRAM 2.4 model (http://projects.tropos.de/capram/capram_24.html).

H₂SO₄: Value measured at 303 K.

Table 5: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

| # | labels | reaction | rate coefficient | reference |
|---|--------|----------|------------------|-----------|
|---|--------|----------|------------------|-----------|

General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca_aero.f90` using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry’s law constants in subroutine `mecca_aero_henry`.

For uptake of X (X = N₂O₅, ClNO₃, or BrNO₃) and subsequent reaction with H₂O, Cl⁻, and Br⁻ in H3201,

H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\text{exf}}(\text{X}) = \frac{k_{\text{mt}}(\text{X}) \times \text{LWC}}{[\text{H}_2\text{O}] + 5 \times 10^2 [\text{Cl}^-] + 3 \times 10^5 [\text{Br}^-]}$$

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt} . The factors only affect the branching between hydrolysis and the halide reac-

tions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[\text{Cl}^-] > 0.1 \text{ M}$ (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\text{H}_2\text{O}]/[\text{Cl}^-]$ is less than 5×10^2 . The ratio $5 \times 10^2 / 3 \times 10^5$ 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 N₂O₅. Here, they are also used for ClNO₃ and BrNO₃.

Table 6: Heterogeneous reactions

| # | labels | reaction | rate coefficient | reference |
|---|--------|----------|------------------|-----------|
|---|--------|----------|------------------|-----------|

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 7: Acid-base and other equilibria

| # | labels | reaction | $K_0[M^{m-n}]$ | $-\Delta H/R[K]$ | reference |
|---|--------|----------|----------------|------------------|-----------|
|---|--------|----------|----------------|------------------|-----------|

Specific notes

Table 8: Aqueous phase reactions

| # | labels | reaction | k_0 [$M^{1-n} s^{-1}$] | $-E_a/R[K]$ | reference |
|---|--------|----------|----------------------------|-------------|-----------|
|---|--------|----------|----------------------------|-------------|-----------|

Specific notes

References

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