

Supplement of manuscript gmd-2021-295

“Simulation of organics in the atmosphere: evaluation of EMACv2.54 with the Mainz Organic Mechanism (MOM) coupled to the ORACLE(v1.0) submodel”

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 3.8u

Date: September 29, 2021

Batch file: mom3d.bat

Replacement file: mom3d

Selected reactions:

“(((Tr && (G || Het) && !I) || St) && !Hg)”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 706

Aqueous phase: 0

All species: 706

Number of reactions in selected mechanism:

Gas phase (Gnnn): 1758

Aqueous phase (Annn): 0

Henry (Hnnn): 0

Photolysis (Jnnn): 360

Aqueous phase photolysis (PHnnn): 0

Heterogeneous (HETnnn): 12

Equilibria (EQnn): 0

Isotope exchange (IEXnnn): 0

Tagging equations (TAGnnn): 0

Dummy (Dnn): 0

All equations: 2130

Table S1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11 * EXP(55./temp)$	Burkholder et al. (2015)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.0E-34 * ((temp/300.) ** (-2.4))$ $* cair$	Burkholder et al. (2015)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2 O_2$	$1.2E-10$	Burkholder et al. (2015)*
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2 O_2$	$8.0E-12 * EXP(-2060./temp)$	Burkholder et al. (2015)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	$k_3rd(temp, cair, 4.4E-32, 1.3,$ $7.5E-11, -0.2, 0.6)$	Burkholder et al. (2015)
G2101	UpStG	$H + O_3 \rightarrow OH + O_2$	$1.4E-10 * EXP(-470./temp)$	Burkholder et al. (2015)
G2102	UpStG	$H_2 + O(^1D) \rightarrow H + OH$	$1.2E-10$	Burkholder et al. (2015)
G2103	UpStG	$OH + O(^3P) \rightarrow H + O_2$	$1.8E-11 * EXP(180./temp)$	Burkholder et al. (2015)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7E-12 * EXP(-940./temp)$	Burkholder et al. (2015)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12 * EXP(-1800./temp)$	Burkholder et al. (2015)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow OH + O_2$	$3.E-11 * EXP(200./temp)$	Burkholder et al. (2015)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14 * EXP(-490./temp)$	Burkholder et al. (2015)
G2108a	UpStG	$HO_2 + H \rightarrow 2 OH$	$7.2E-11$	Burkholder et al. (2015)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	$6.9E-12$	Burkholder et al. (2015)
G2108c	UpStG	$HO_2 + H \rightarrow O(^3P) + H_2O$	$1.6E-12$	Burkholder et al. (2015)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11 * EXP(250./temp)$	Burkholder et al. (2015)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_H02_H02	Burkholder et al. (2015)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$1.63E-10 * EXP(60./temp)$	Burkholder et al. (2015)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$1.8E-12$	Burkholder et al. (2015)
G3100	UpStGN	$N + O_2 \rightarrow NO + O(^3P)$	$1.5E-11 * EXP(-3600./temp)$	Burkholder et al. (2015)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11 * EXP(110./temp)$	Burkholder et al. (2015)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow 2 NO$	$7.259E-11 * EXP(20./temp)$	Burkholder et al. (2015)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	$4.641E-11 * EXP(20./temp)$	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.0E-12 * EXP(-1500./temp)$	Burkholder et al. (2015)
G3104	UpStGN	$NO + N \rightarrow O(^3P) + N_2$	$2.1E-11 * EXP(100./temp)$	Burkholder et al. (2015)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.1E-12 * EXP(210./temp)$	Burkholder et al. (2015)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13 * EXP(-2450./temp)$	Burkholder et al. (2015)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12 * EXP(220./temp)$	Burkholder et al. (2015)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11 * EXP(170./temp)$	Burkholder et al. (2015)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_N03_N02	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_N03_N02 / (5.8E-27 * EXP(10840./$ $temp))$	Burkholder et al. (2015)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$k_{3rd}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6, 3.6\text{E-}11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.3\text{E-}12 * \text{EXP}(270./\text{temp})$	Burkholder et al. (2015)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$k_{3rd}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0, 2.8\text{E-}11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$k_{\text{NO2_HO2}}$	Burkholder et al. (2015)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E-}12$	Burkholder et al. (2015)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11 * \text{EXP}(-390./\text{temp})$	Burkholder et al. (2015)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$k_{\text{HNO3_OH}}$	Dulitz et al. (2018)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$k_{\text{NO2_HO2}} / (2.1\text{E-}27 * \text{EXP}(10900./\text{temp}))$	Burkholder et al. (2015)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E-}12 * \text{EXP}(380./\text{temp})$	Burkholder et al. (2015)
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E-}12 * \text{EXP}(-710./\text{temp})$	Kohlmann and Poppe (1999)
G3210	TrGN	$\text{NH}_2 + \text{O}_3 \rightarrow \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12 * \text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E-}07 * \text{EXP}(-628./\text{temp})$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$*\text{temp}^{**}(-1.32)$ $9.4\text{E-}09 * \text{EXP}(-356./\text{temp})$ $*\text{temp}^{**}(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12 * ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11 * ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11 * ((\text{temp}/298.)^{**}(-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11 * ((\text{temp}/298.)^{**}(-2.0))$	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	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	$8.0\text{E-}11 * \text{EXP}(-500./\text{temp})$	Kohlmann and Poppe (1999)
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E-}12 * \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$	$1.0\text{E-}12 * \text{EXP}(-1000./\text{temp})$	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	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11 * \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14 * \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4100	UpStG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow .75 \text{CH}_3 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	$1.75\text{E-}10$	Burkholder et al. (2015)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	$1.85\text{E-}20 * \text{EXP}(2.82 * \text{LOG}(\text{temp}) - 987./\text{temp})$	Atkinson (2003)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{HCHO} + .85 \text{HO}_2 + .15 \text{CH}_3\text{O} + \text{H}_2\text{O}$	$6.38\text{E-}18 * (\text{temp}^{**2}) * \text{EXP}(144./\text{temp})$	Atkinson et al. (2006)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$3.8\text{E-}13 * \text{EXP}(780./\text{temp}) / (1.+1./498.*\text{EXP}(1160./\text{temp}))$	Atkinson et al. (2006)
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$3.8\text{E-}13 * \text{EXP}(780./\text{temp}) / (1.+498.*\text{EXP}(-1160./\text{temp}))$	Atkinson et al. (2006)
G4104a	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	$2.3\text{E-}12 * \text{EXP}(360./\text{temp}) * (1.-\text{beta}_{\text{CH3NO3}})$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$	$2.3\text{E-}12 * \text{EXP}(360./\text{temp}) * \text{beta}_{\text{CH3NO3}}$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$	1.2E-12	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{O}_2$	$7.4\text{E-}13 * \text{EXP}(-520./\text{temp}) * \text{R02} * 2.$	Atkinson et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$(k_{\text{CH3O2}} - 7.4\text{E-}13 * \text{EXP}(-520./\text{temp})) * \text{R02} * 2.$	Atkinson et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{CH}_3\text{O}_2 + .4 \text{HCHO} + .4 \text{OH} + \text{H}_2\text{O}$	$k_{\text{CH3OOH_OH}}$	Wallington et al. (2018)
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	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 * \text{EXP}(-1900./\text{temp})$	Burkholder et al. (2015)*
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)
G4112	UpStG	$\text{CO} + \text{O}(^3\text{P}) \rightarrow \text{CO}_2$	$6.60\text{E-}33 * \text{EXP}(-1103./\text{temp})$	Roble (1995)
G4113	UpStG	$\text{CH}_4 + \text{O}(^3\text{P}) \rightarrow .51 \text{CH}_3 + .51 \text{OH} + .49 \text{CH}_3\text{O} + .49 \text{H}$	$6.03\text{E-}18 * \text{temp}^{**}(2.17) * \text{EXP}(-3619./\text{temp})$	Roble (1995), Garton et al. (2003), Espinosa-Garcia and Garcia-Bernáldez (2000)
G4114	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	$k_{\text{NO2_CH3O2}}$	Burkholder et al. (2015)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$k_{\text{NO2_CH3O2}} / (9.5\text{E-}29 * \text{EXP}(11234./\text{temp}))$	Burkholder et al. (2015)*
G4116	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$	3.00E-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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 2.6\text{E-}29, 2.8, 3.3\text{E-}11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/900.), \text{SP}))$	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	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E-}16*\text{exp}(-1000./\text{temp})$	Burkholder et al. (2015)
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	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	1.2E-12	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(\text{k_CH302}*5.5\text{E-}12)**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(\text{k_CH302}*5.7\text{E-}14*\text{EXP}(750./\text{temp}))**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*\text{k_CH300H_OH}$	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$\text{k_rohro} + \text{k_s*f_sooh*f_soh}$	Taraborrelli (2010)*
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$2.*\text{k_rohro} + \text{k_s*f_soh*f_soh}$	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	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E+}14*\text{EXP}(-10000/\text{temp})$	see note*
G4135	StTrG	$\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$	$\text{k_CH200_N02}*3.6\text{E-}6$	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_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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	k_N02_CH3O2	see note*
G4149	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$	$k_{\text{N02_CH3O2}} / (9.5\text{E-}29 * \text{EXP}(11234./\text{temp}))$	Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E-}13 * \text{EXP}(-650./\text{temp}) * f_{\text{soh}}$	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	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{ HCHO} + .956 \text{ H} + .044 \text{ CH}_3\text{O} + \text{O}_2$	$5.1\text{E-}12 * \text{exp}(-210./\text{temp})$	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	$\text{HCHO} + \text{O}({}^3\text{P}) \rightarrow .7 \text{ OH} + .7 \text{ CO} + .3 \text{ H} + .3 \text{ CO}_2 + \text{HO}_2$	$3.4\text{E-}11 * \text{EXP}(-1600./\text{temp})$	Burkholder et al. (2015)
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)
G4159	TrGN	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$	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	$\text{HCN} + \text{O}({}^3\text{P}) \rightarrow \text{H} + \text{NCO}$	$1.0\text{E-}11 * \text{EXP}(-4000./\text{temp})$	Burkholder et al. (2015)*
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.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	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$	Atkinson et al. (2006), Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G42003	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	$7.5E-13*EXP(700./temp)$	Burkholder et al. (2015)
G42004a	TrGCN	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	$2.55E-12*EXP(380./temp)*(1.-beta_{C2H5NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$C_2H_5O_2 + NO \rightarrow C_2H_5ONO_2$	$2.55E-12*EXP(380./temp)*beta_{C2H5NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42005	TrGCN	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	$2.3E-12$	Wallington et al. (2018)
G42006	TrGC	$C_2H_5O_2 \rightarrow .8 CH_3CHO + .6 HO_2 + .2 C_2H_5OH$	$2.*(7.6E-14*k_{CH3O2})*(0.5)*R02$	Sander et al. (2019), Atkinson et al. (2006)
G42007a	TrGC	$C_2H_5OOH + OH \rightarrow C_2H_5O_2 + H_2O$	$0.6*k_{CH3OOH_OH}$	Sander et al. (2019)
G42007b	TrGC	$C_2H_5OOH + OH \rightarrow CH_3CHO + OH$	$k_{s* f_{sooh}}$	Sander et al. (2019)
G42008a	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O) + H_2O$	$4.4E-12*EXP(365./temp)*0.95$	Atkinson et al. (2006)
G42008b	TrGC	$CH_3CHO + OH \rightarrow HCOCH_2O_2 + H_2O$	$4.4E-12*EXP(365./temp)*0.05$	Atkinson et al. (2006)
G42009	TrGCN	$CH_3CHO + NO_3 \rightarrow CH_3C(O) + HNO_3$	KN03AL	Rickard and Pascoe (2009)
G42010	TrGC	$CH_3COOH + OH \rightarrow CH_3 + CO_2 + H_2O$	$4.0E-14*EXP(850./temp)$	Atkinson et al. (2006)*
G42011a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow OH + CH_3 + CO_2$	$5.20E-13*EXP(980./temp)*1.507*0.61$	Groß et al. (2014)
G42011b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	$5.20E-13*EXP(980./temp)*1.507*0.23$	Groß et al. (2014)
G42011c	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	$5.20E-13*EXP(980./temp)*1.507*0.16$	Groß et al. (2014)
G42012	TrGCN	$CH_3C(O)OO + NO \rightarrow CH_3 + CO_2 + NO_2$	$8.1E-12*EXP(270./temp)$	Tyndall et al. (2001a)
G42013	TrGCN	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_{CH3C03_NO2}	Burkholder et al. (2015)*
G42014	TrGCN	$CH_3C(O)OO + NO_3 \rightarrow CH_3 + NO_2 + CO_2$	$4.E-12$	Canosa-Mas et al. (1996)
G42017a	TrGC	$CH_3C(O)OO \rightarrow CH_3 + CO_2$	$k1_{R02RC03}*0.9$	Sander et al. (2019)
G42017b	TrGC	$CH_3C(O)OO \rightarrow CH_3COOH$	$k1_{R02RC03}*0.1$	Sander et al. (2019)
G42018	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	$0.6*k_{CH3OOH_OH}$	Rickard and Pascoe (2009)*
G42020	TrGCN	$PAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	$3.00E-14$	Rickard and Pascoe (2009)
G42021	TrGCN	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_{PAN_M}	Burkholder et al. (2015)*
G42022a	TrGC	$C_2H_2 + OH \rightarrow GLYOX + OH$	$k_{3rd}(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.71$	Burkholder et al. (2015)*
G42022b	TrGC	$C_2H_2 + OH \rightarrow HCOOH + CO + HO_2$	$k_{3rd}(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.29$	Burkholder et al. (2015)*
G42023a	TrGC	$HOCH_2CHO + OH \rightarrow HOCH_2CO + H_2O$	$8.00E-12*0.80$	Atkinson et al. (2006)
G42023b	TrGC	$HOCH_2CHO + OH \rightarrow HOCHCHO + H_2O$	$8.00E-12*0.20$	Atkinson et al. (2006)
G42024a	TrGC	$HOCH_2CO + O_2 \rightarrow HOCH_2CO_3$	$5.1E-12*(1.-1./(1+1.85E-18*cair))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42024b	TrGC	$HOCH_2CO + O_2 \rightarrow OH + HCHO + CO_2$	$5.1E-12*1./(1+1.85E-18*cair)$	Atkinson et al. (2006), Beyersdorf et al. (2010)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G42025	TrGC	$\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Sander et al. (2019)
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	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	$k1_R02RC03*0.9$	Sander et al. (2019)
G42027b	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$k1_R02RC03*0.1$	Sander et al. (2019)
G42028a	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	KAPH02*rc03_oh	Sander et al. (2019), 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*rc03_ooH	Sander et al. (2019), 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*rc03_o3	Sander et al. (2019), 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	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KR02NO3*1.60	Rickard and Pascoe (2009)
G42032	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{HCHO} + .09 \text{CO}_2 + .91 \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	$k_co2h+k_s*f_soh*f_co2h$	Sander et al. (2019)
G42033a	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Sander et al. (2019)
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	$k_s*f_soh*f_co2h$	Sander et al. (2019)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42035	TrGCN	$\text{PHAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_s*f_soh*f_cpan+k_rohro$	Sander et al. (2019)
G42036	TrGC	$\text{GLYOX} + \text{OH} \rightarrow \text{HCOCO} + \text{H}_2\text{O}$	$3.1E-12*EXP(340./temp)$	Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013)
G42037	TrGCN	$\text{GLYOX} + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42038a	TrGC	$\text{HCOCO} \rightarrow \text{CO} + \text{CO} + \text{HO}_2$	$7.E11*EXP(-3160./temp) + 5.E-12*c(ind_02)$	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	$\text{HCOCO} \rightarrow \text{HCOCO}_3$	$5.E-12*c(ind_02)*3.2*exp(-550./temp)$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	$\text{HCOCO} \rightarrow \text{OH} + \text{CO} + \text{CO}_2$	$5.E-12*c(ind_02) * (1.-3.2*exp(-550./temp))$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	$\text{HCOCO}_3 \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2$	$k1_R02RC03*0.9$	Sander et al. (2019)
G42039b	TrGC	$\text{HCOCO}_3 \rightarrow \text{HCOCO}_2\text{H}$	$k1_R02RC03*0.1$	Sander et al. (2019)
G42040	TrGC	$\text{HCOCO}_3 + \text{HO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02	Feierabend et al. (2008), Sander et al. (2019)
G42041	TrGCN	$\text{HCOCO}_3 + \text{NO} \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G42042	TrGCN	$\text{HCOCO}_3 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	$\text{KR02N03} \cdot 1.60$	Rickard and Pascoe (2009)
G42043	TrGCN	$\text{HCOCO}_3 + \text{NO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_3 + \text{CO}_2$	k_CH3C03_N02	Orlando and Tyndall (2001), Sander et al. (2019)
G42044	TrGC	$\text{HCOCO}_2\text{H} + \text{OH} \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{k_co2h} + \text{k_t*f_o*f_co2h}$	Sander et al. (2019)
G42045a	TrGC	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3 + \text{H}_2\text{O}$	$0.6 \cdot \text{k_CH300H_OH}$	Sander et al. (2019)
G42045b	TrGC	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{CO} + \text{CO}_2 + \text{H}_2\text{O} + \text{OH}$	k_t*f_o*f_co2h	Sander et al. (2019)
G42046	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 \rightarrow .6 \text{HOCH}_2\text{CH}_2\text{O} + .2 \text{HOCH}_2\text{CHO} + .2 \text{ETHGLY}$	$2 \cdot (7.8\text{E}-14 \cdot \text{EXP}(1000./\text{temp})) \cdot \text{k_CH302} \cdot (.5) \cdot \text{R02}$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow .25 \text{HO}_2 + .5 \text{HCHO} + .75 \text{HOCH}_2\text{CH}_2\text{O} + \text{NO}_2$	$\text{KR02N0} \cdot (1. - \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G42048	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{ETHOHNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair})$	Sander et al. (2019)
G42049a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HYETHO2H}$	$1.53\text{E}-13 \cdot \text{EXP}(1300./\text{temp}) \cdot (1. - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G42049b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$1.53\text{E}-13 \cdot \text{EXP}(1300./\text{temp}) \cdot \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)
G42050	TrGCN	$\text{ETHOHNO}_3 + \text{OH} \rightarrow .93 \text{NO}_3\text{CH}_2\text{CHO} + .93 \text{HO}_2 + .07 \text{HOCH}_2\text{CHO} + .07 \text{NO}_2 + \text{H}_2\text{O}$	$\text{k_s} \cdot (\text{f_soh} \cdot \text{f_ch2ono2} + \text{f_ono2} \cdot \text{f_pch2oh}) + \text{k_rohro}$	Sander et al. (2019)
G42051a	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot \text{k_CH300H_OH}$	Rickard and Pascoe (2009)*
G42051b	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$	$\text{k_s} \cdot \text{f_soh} \cdot \text{f_pch2oh}$	Sander et al. (2019)
G42051c	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$\text{k_s} \cdot \text{f_soh} \cdot \text{f_pch2oh} + \text{k_rohro}$	Sander et al. (2019)
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	$\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$2 \cdot \text{k_s} \cdot \text{f_soh} \cdot \text{f_pch2oh} + 2 \cdot \text{k_rohro}$	Sander et al. (2019)
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_R02p0R02	Sander et al. (2019)
G42055a	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CHO}$	$\text{KR02H02}(2) \cdot \text{rcoch2o2_ooh}$	Sander et al. (2019)
G42055b	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(2) \cdot \text{rcoch2o2_oh}$	Sander et al. (2019)
G42056a	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{KR02N0} \cdot (1. - \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G42056b	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair})$	Sander et al. (2019)
G42057	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2019)
G42058a	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2$	$0.6 \cdot \text{k_CH300H_OH}$	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G42058b	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH}$.8*8.E-12	Sander et al. (2019)*
G42058c	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	$k_{\text{s*f_sooh*f_cho}}$	Sander et al. (2019)
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	Sander et al. (2019)
G42061	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	KR02NO3*1.60	Sander et al. (2019)
G42062a	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 2 \text{OH} + \text{HCHO} + \text{CO}_2$	KAPH02*rc03_oh	Sander et al. (2019)
G42062b	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	KAPH02*rc03_ooH	Sander et al. (2019)
G42062c	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rc03_o3	Sander et al. (2019)
G42063a	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	$k_{1_R02RC03*0.9}$	Sander et al. (2019)
G42063b	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$	$k_{1_R02RC03*0.1}$	Sander et al. (2019)
G42064a	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$2.*0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G42064b	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f_sooh*f_co2h}}$	Sander et al. (2019)
G42065	TrGC	$\text{HOOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCO}_2\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f_sooh*f_co2h+k_co2h}}$	Sander et al. (2019)
G42066	TrGC	$\text{CH}_2\text{CO} + \text{OH} \rightarrow .6 \text{HCHO} + .6 \text{HO}_2 + .6 \text{CO} + .4 \text{HOOCH}_2\text{CO}_2\text{H}$	$2.8\text{E-}12*\exp(510./\text{temp})$	Baulch et al. (2005), Sander et al. (2019)
G42067a	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{OH}$	$(k_{\text{t*f_tooh*f_toh}} + k_{\text{rohro}})$	Sander et al. (2019)
G42067b	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$	$0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G42068	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$3.46\text{E}12*\text{EXP}(-12500./(1.98*\text{temp}))$	Hermans et al. (2005), Sander et al. (2019)
G42069	TrGC	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$	$3.46\text{E}12*\text{EXP}(-12500./(1.98*\text{temp})) / (6.34\text{E}26*\text{EXP}(-14700./(1.98*\text{temp})))$	Hermans et al. (2005), Sander et al. (2019)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{CH}_3\text{CHOHOOH} + .3 \text{CH}_3\text{COOH} + .2 \text{CH}_3 + .2 \text{HCOOH} + .2 \text{OH}$	$5.6\text{E-}15*\text{EXP}(2300./\text{temp})$	Sander et al. (2019)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	$k_{1_R02s0R02}$	Sander et al. (2019)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KR02NO	Sander et al. (2019)
G42073	TrGCN	$\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$	$6.7\text{E-}13*\text{EXP}(-395./\text{temp})$	Atkinson et al. (2006)
G42074a	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f_ch2ono2*f_cho}}$	Paulot et al. (2009a), Sander et al. (2019)*
G42074b	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{H}_2\text{O}$	$k_{\text{t*f_o*f_ch2ono2*3.}}$	Paulot et al. (2009a), Sander et al. (2019)*
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	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G42078	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$	$k_{1_R02RC03}$	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	9.50E-13*EXP(-650./temp)	Sander et al. (2019)*
G42083a	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	5.1E-12*(1. - 1./(1.+ 9.4E-18*cair))	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42083b	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$	5.1E-12*1./(1.+9.4E-18*cair)	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{ C}_2\text{H}_5\text{O}_2 + .95 \text{ HO}_2 + .05 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	3.0E-12*EXP(20./temp)	Sander et al. (2019), Atkinson et al. (2006)
G42085a	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$	8.1E-13*EXP(-1080./temp)*0.40	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42085b	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$	8.1E-13*EXP(-1080./temp)*(1.-0.40)	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$	2.54E-10*EXP(-24./temp)*0.0269*EXP(137./temp)	Strekowski et al. (2010)
G42086b	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{ H} + \text{CO} + \text{HCN}$	2.54E-10*EXP(-24./temp)*0.16	Strekowski et al. (2010)*
G42086c	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{ CH}_3 + .5 \text{ NCO} + .5 \text{ NCCH}_2\text{O}_2 + .5 \text{ OH}$	2.54E-10*EXP(-24./temp)*(1.-(0.16+ 0.0269*EXP(137./temp)))	Strekowski et al. (2010)*
G42087	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N0	see note*
G42088	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$	KR02H02(2)	see note*
G42089a	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{HCHO}$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), 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	Sander et al. (2019), So et al. (2014)
G42090	TrGC	$\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G42091	TrGC	$\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (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	Sander et al. (2019)
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	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G43001a	TrGC	$C_3H_6 + O_3 \rightarrow HCHO + .16 CH_3CHOHO_2 + .50 OH + .50 HCOCH_2O_2 + .05 CH_2CO + .09 CH_3OH + .09 CO + .2 CH_4 + .2 CO_2$	$5.5E-15*EXP(-1880./temp)*.57$	Atkinson et al. (2006)*
G43001b	TrGC	$C_3H_6 + O_3 \rightarrow CH_3CHO + CH_2OO^*$	$5.5E-15*EXP(-1880./temp)*.43$	Atkinson et al. (2006)*
G43002	TrGC	$C_3H_6 + OH \rightarrow HYPROPO_2$	$k_3rd_iupac(temp, cair, 8.6E-27, 3.5, 3.E-11, 1., 0.5)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$C_3H_6 + NO_3 \rightarrow PRONO_3BO_2$	$4.6E-13*EXP(-1155./temp)$	Wallington et al. (2018)
G43004	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	$1.9E-13*EXP(1300./temp)$	Atkinson (1997)*
G43005a	TrGCN	$iC_3H_7O_2 + NO \rightarrow CH_3COCH_3 + HO_2 + NO_2$	$2.7E-12*EXP(360./temp)*(1.-alpha_AN(3, 2, 0, 0, 0, temp, cair))$	Wallington et al. (2018)
G43005b	TrGCN	$iC_3H_7O_2 + NO \rightarrow iC_3H_7ONO_2$	$2.7E-12*EXP(360./temp)*alpha_AN(3, 2, 0, 0, 0, temp, cair)$	Wallington et al. (2018)
G43006	TrGC	$iC_3H_7O_2 \rightarrow .8 CH_3COCH_3 + .2 IPROPOL + .6 HO_2$	$2.*(1.6E-12*EXP(-2200./temp)*k_CH302)**(.5)*R02$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	$iC_3H_7OOH + OH \rightarrow iC_3H_7O_2 + H_2O$	$0.6*k_CH300H_OH$	Sander et al. (2019)
G43007b	TrGC	$iC_3H_7OOH + OH \rightarrow CH_3COCH_3 + H_2O + OH$	k_t*f_tooh	Sander et al. (2019)
G43008	TrGC	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	$1.9E-13*EXP(1300./temp)$	Atkinson (1997)*
G43009a	TrGCN	$C_3H_7O_2 + NO \rightarrow C_2H_5CHO + HO_2 + NO_2$	$2.7E-12*EXP(360./temp)*(1.-alpha_AN(3, 1, 0, 0, 0, temp, cair))$	Wallington et al. (2018)
G43009b	TrGCN	$C_3H_7O_2 + NO \rightarrow C_3H_7ONO_2$	$2.7E-12*EXP(360./temp)*alpha_AN(3, 1, 0, 0, 0, temp, cair)$	Wallington et al. (2018)
G43010	TrGC	$C_3H_7O_2 \rightarrow .8 CH_3COCH_3 + .2 NPROPOL + .6 HO_2$	$2.*(k_CH302*3.E-13)**(.5)*R02$	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), Sander et al. (2019)
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), Sander et al. (2019)
G43013a	TrGCN	$CH_3COCH_2O_2 + NO \rightarrow CH_3C(O) + HCHO + NO_2$	$2.9E-12*EXP(300./temp)*(1.-alpha_AN(4, 1, 1, 0, 0, temp, cair))$	Burkholder et al. (2015)
G43013b	TrGCN	$CH_3COCH_2O_2 + NO \rightarrow NOA$	$2.9E-12*EXP(300./temp)*alpha_AN(4, 1, 1, 0, 0, temp, cair)$	Burkholder et al. (2015)
G43014	TrGC	$CH_3COCH_2O_2 \rightarrow .3 CH_3C(O) + .3 HCHO + .5 MGLYOX + .2 CH_3COCH_2OH$	$k1_R02p0R02$	Orlando and Tyndall (2012)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G43015a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H_OH}}$	see note*
G43015b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f_sooh*f_co}}$	Sander et al. (2019)
G43016	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$1.6\text{E-}12 \cdot \text{EXP}(305./\text{temp})$	Atkinson et al. (2006)
G43017	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{ CH}_3 + .6 \text{ CH}_3\text{C}(\text{O}) + 1.4 \text{ CO} + \text{H}_2\text{O}$	$1.9\text{E-}12 \cdot \text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13 \cdot \text{EXP}(-230./\text{temp})$	Wallington et al. (2018)
G43021	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43022	TrGC	$\text{HYPROPO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	k1_R02sOR02	Rickard and Pascoe (2009)
G43023a	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{HYPROPO}_2\text{H}$	$\text{KR02H02}(3) \cdot (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G43023b	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(3) \cdot \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)
G43024a	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G43024b	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{PROPOLNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G43025	TrGCN	$\text{HYPROPO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43026a	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{HYPROPO}_2$	$0.6 \cdot k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G43026b	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{\text{s*f_soh*f_pch2oh}} + k_{\text{t*f_tooh*f_pch2oh}})$	Sander et al. (2019)
G43027	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{HO}_2 \rightarrow \text{PR}_2\text{O}_2\text{HNO}_3$	KR02H02(3)	Rickard and Pascoe (2009)
G43028	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43029	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43030a	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{PRONO}_3\text{BO}_2$	$0.6 \cdot k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G43030b	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{\text{t*f_tooh*f_ch2ono2}}$	Sander et al. (2019)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Rickard and Pascoe (2009)
G43032	TrGCN	$\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$	$(k_{\text{s*f_co*f_ono2}} + k_{\text{p*f_co}})$	Sander et al. (2019)
G43033	TrGC	$\text{HOCH}_2\text{COCHO} + \text{OH} \rightarrow .8609 \text{ HOCH}_2\text{CO} + .8609 \text{ CO} + .1391 \text{ HCOCOCHO} + .1391 \text{ HO}_2$	$(1.9\text{E-}12 \cdot \text{EXP}(575./\text{temp}) + k_{\text{s*f_soh*f_co}})$	Sander et al. (2019)
G43034	TrGCN	$\text{HOCH}_2\text{COCHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Sander et al. (2019)
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E-}14 \cdot \text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Sander et al. (2019)
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_R02pOR02	Sander et al. (2019)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$\text{KR02H02}(3) \cdot \text{rcoch2o2_ooh}$	Sander et al. (2019)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{KR02H02}(3) \cdot \text{rcoch2o2_oh}$	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{\text{t}}*f_{\text{co}}*f_{\text{o}}$	Sander et al. (2019)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}}*f_{\text{sooh}}*f_{\text{co}}$	Sander et al. (2019)*
G43040c	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G43041	TrGCN	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Sander et al. (2019)
G43042	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO}$	k1_R02pOR02	Sander et al. (2019)
G43043a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$\text{KR02H02(3)}*r_{\text{coch2o2_ooh}}$	Sander et al. (2019)
G43043b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{OH}$	$\text{KR02H02(3)}*r_{\text{coch2o2_oh}}$	Sander et al. (2019)
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	Sander et al. (2019)*
G43045a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCHO} + \text{OH}$	$k_{\text{s}}*f_{\text{sooh}}*f_{\text{co}}$	Sander et al. (2019)
G43045b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{O}_2$	$.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G43045c	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E-}12*\text{EXP}(305./\text{temp})$	Sander et al. (2019)*
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), Sander et al. (2019)
G43047	TrGCN	$\text{PROPOLNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{\text{t}}*f_{\text{ono2}}*f_{\text{pch2oh}}+k_{\text{s}}*f_{\text{soh}}*f_{\text{ch2ono2}}$	Sander et al. (2019)
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	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E-}13*\text{EXP}(-650./\text{temp})*f_{\text{co}}$	Sander et al. (2019)*
G43051a	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G43051b	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}}*f_{\text{sooh}}$	Sander et al. (2019)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{pch2oh}}$	Sander et al. (2019)*
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	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}}*0.9$	Sander et al. (2019)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	$k1_{\text{R02RC03}}*0.1$	Sander et al. (2019)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{co3_oh}}$	Sander et al. (2019), Groß et al. (2014)
G43055b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$	$\text{KAPH02}*r_{\text{co3_ooh}}$	Sander et al. (2019), Groß et al. (2014)
G43055c	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02}*r_{\text{co3_o3}}$	Sander et al. (2019), 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	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	$k_{\text{CH3C03_N02}}$	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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G43059	TrGC	$C_2H_5CO_2H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	$k_{co2h+k_p+k_{s*f_{co2h}}}$	Sander et al. (2019)*
G43060a	TrGC	$C_2H_5CO_3H + OH \rightarrow C_2H_5CO_3 + H_2O$	$0.6*k_{CH300H_{OH}}$	Sander et al. (2019)
G43060b	TrGC	$C_2H_5CO_3H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	$k_{s*f_{co2h}+k_p}$	Sander et al. (2019)*
G43061	TrGCN	$PPN + OH \rightarrow CH_3CHO + CO_2 + NO_2 + H_2O$	$k_{s*f_{cpan}+k_p}$	Sander et al. (2019)*
G43062	TrGC	$CH_3COCO_3H + OH \rightarrow CH_3COCO_3 + H_2O$	$0.6*k_{CH300H_{OH}}$	Sander et al. (2019)
G43063a	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3C(O) + CO_2 + OH$	$KAPH02*rco3_{oh}$	Sander et al. (2019)
G43063b	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3COCO_3H$	$KAPH02*(rco3_{ooh}+rco3_{o3})$	Sander et al. (2019)
G43064	TrGCN	$CH_3COCO_3 + NO \rightarrow CH_3C(O) + CO_2 + NO_2$	KAPNO	Sander et al. (2019)
G43065	TrGCN	$CH_3COCO_3 + NO_2 \rightarrow CH_3C(O) + CO_2 + NO_3$	$k_{CH3C03_{NO2}}$	Sander et al. (2019)*
G43066	TrGCN	$CH_3COCO_3 + NO_3 \rightarrow CH_3C(O)OO + CO_2 + NO_2$	$KR02NO3*1.74$	Sander et al. (2019)
G43067	TrGC	$CH_3COCO_3 \rightarrow CH_3C(O)OO + CO_2$	$k1_{R02RC03}$	Sander et al. (2019)
G43068	TrGC	$HCOCOCHO + OH \rightarrow 3 CO + HO_2$	$2.*k_{t*f_{co*f_o}}$	Sander et al. (2019)
G43069	TrGC	$IPROPOL + OH \rightarrow CH_3COCH_3 + HO_2 + H_2O$	$2.6E-12*EXP(200./temp)$	Atkinson et al. (2006)
G43070a	TrGC	$NPROPOL + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$	$4.6E-12*EXP(70./temp)*(k_{s*f_{soh}}/(k_p+k_{s*f_{pch2oh}+k_{s*f_{soh}}}))$	Atkinson et al. (2006), Sander et al. (2019)*
G43070b	TrGC	$NPROPOL + OH \rightarrow HYPROPO2 + H_2O$	$4.6E-12*EXP(70./temp)*((k_p+k_{s*f_{pch2oh}})/(k_p+k_{s*f_{pch2oh}+k_{s*f_{soh}}}))$	Atkinson et al. (2006), Sander et al. (2019)*
G43071a	TrGC	$CH_2CHCH_2OH + OH \rightarrow HCOOH + OH + CH_3CHO$	$k_{CH2CHOH_{OH_{HCOOH}}}$	Sander et al. (2019), So et al. (2014)*
G43072	TrGC	$CH_2CHCH_2OH + HCOOH \rightarrow C_2H_5CHO + HCOOH$	$k_{CH2CHOH_{HCOOH}}$	Sander et al. (2019), da Silva (2010)*
G43073	TrGC	$C_2H_5CHO + HCOOH \rightarrow CH_2CHCH_2OH + HCOOH$	$k_{ALD_{HCOOH}}$	Sander et al. (2019), da Silva (2010)*
G43074	TrGC	$HCOCOCH_2OOH + OH \rightarrow HCOCO + CO + HO_2 + OH$	$k_{s*f_{sooh*f_{co}}+6*k_{CH300H_{OH}}}$	Sander et al. (2019)*
G43202	TrGTerC	$HCOCH_2CHO + OH \rightarrow HCOCH_2CO_3$	$4.29E-11$	Rickard and Pascoe (2009)
G43203	TrGTerCN	$HCOCH_2CHO + NO_3 \rightarrow HCOCH_2CO_3 + HNO_3$	$2.*KN03AL*2.4$	Rickard and Pascoe (2009)
G43204a	TrGTerC	$HCOCH_2CO_3 \rightarrow HCOCH_2O_2 + CO_2$	$k1_{R02RC03*0.9}$	Sander et al. (2019)
G43204b	TrGTerC	$HCOCH_2CO_3 \rightarrow HCOCH_2CO_2H$	$k1_{R02RC03*0.1}$	Sander et al. (2019)
G43205	TrGTerCN	$HCOCH_2CO_3 + NO \rightarrow HCOCH_2O_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43206	TrGTerCN	$HCOCH_2CO_3 + NO_2 \rightarrow C_3PAN2$	$k_{CH3C03_{NO2}}$	Rickard and Pascoe (2009)
G43207a	TrGTerC	$HCOCH_2CO_3 + HO_2 \rightarrow HCOCH_2CO_3H$	$KAPH02*rco3_{ooh}$	Rickard and Pascoe (2009)
G43207b	TrGTerC	$HCOCH_2CO_3 + HO_2 \rightarrow HCOCH_2CO_2H + O_3$	$KAPH02*rco3_{o3}$	Rickard and Pascoe (2009)
G43207c	TrGTerC	$HCOCH_2CO_3 + HO_2 \rightarrow HCOCH_2O_2 + CO_2 + OH$	$KAPH02*rco3_{oh}$	Rickard and Pascoe (2009)
G43210	TrGTerCN	$C_3PAN2 \rightarrow HCOCH_2CO_3 + NO_2$	k_{PAN_M}	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G43211	TrGTerCN	$C_3PAN2 + OH \rightarrow GLYOX + CO + NO_2$	2.10E-11	Rickard and Pascoe (2009)
G43212	TrGTerC	$HCOCH_2CO_2H + OH \rightarrow HCOCH_2O_2 + CO_2$	2.14E-11	Rickard and Pascoe (2009)
G43213a	TrGTerC	$HOC_2H_4CO_3 \rightarrow HOCH_2CH_2O_2 + CO_2$	k1_R02RC03*0.9	Sander et al. (2019)
G43213b	TrGTerC	$HOC_2H_4CO_3 \rightarrow HOC_2H_4CO_2H$	k1_R02RC03*0.1	Sander et al. (2019)
G43214	TrGTerCN	$HOC_2H_4CO_3 + NO \rightarrow HOCH_2CH_2O_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow HOC_2H_4CO_3H$	KAPH02*rco3_ooH	Rickard and Pascoe (2009)
G43215b	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow HOCH_2CH_2O_2 + CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G43215c	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow HOC_2H_4CO_2H + O_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G43218	TrGTerCN	$HOC_2H_4CO_3 + NO_2 \rightarrow C_3PAN1$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G43219	TrGTerC	$HOC_2H_4CO_2H + OH \rightarrow HOCH_2CH_2O_2 + CO_2$	1.39E-11	Rickard and Pascoe (2009)
G43220	TrGTerC	$HOC_2H_4CO_3H + OH \rightarrow HOC_2H_4CO_3$	1.73E-11	Rickard and Pascoe (2009)
G43221	TrGTerCN	$C_3PAN1 \rightarrow HOC_2H_4CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G43222	TrGTerCN	$C_3PAN1 + OH \rightarrow HOCH_2CHO + CO + NO_2$	4.51E-12	Rickard and Pascoe (2009)
G43223	TrGTerC	$HCOCH_2CO_3H + OH \rightarrow HCOCH_2O_2 + CO_2 + H_2O$	2.49E-11	Rickard and Pascoe (2009)*
G43415	TrGAroC	$C_3DIALOOH + OH \rightarrow HCOCOCHO + OH$	1.44E-10	Rickard and Pascoe (2009)
G43418a	TrGAroC	$C_3DIALO_2 + HO_2 \rightarrow C_3DIALOOH$	KR02H02(3)*(rco3_ooH+rco3_o3)	Rickard and Pascoe (2009)
G43418b	TrGAroC	$C_3DIALO_2 + HO_2 \rightarrow GLYOX + CO + HO_2 + OH$	KR02H02(3)*rco3_oh	Rickard and Pascoe (2009)
G43419	TrGAroCN	$C_3DIALO_2 + NO \rightarrow GLYOX + CO + HO_2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G43420	TrGAroCN	$C_3DIALO_2 + NO_3 \rightarrow GLYOX + CO + HO_2 + NO_2$	KR02NO3	Rickard and Pascoe (2009)*
G43421	TrGAroC	$C_3DIALO_2 \rightarrow GLYOX + CO + HO_2$	k1_R02sOR02	Rickard and Pascoe (2009)*
G43422a	TrGAroC	$HCOCOHC03 + HO_2 \rightarrow GLYOX + CO_2 + HO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G43422b	TrGAroC	$HCOCOHC03 + HO_2 \rightarrow HCOCOHC03H$	KAPH02*(rco3_ooH+rco3_o3)	Rickard and Pascoe (2009)
G43424	TrGAroCN	$HCOCOHC03 + NO \rightarrow GLYOX + CO_2 + HO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43425	TrGAroCN	$HCOCOHC03 + NO_2 \rightarrow HCOCOHPAN$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G43426	TrGAroCN	$HCOCOHC03 + NO_3 \rightarrow GLYOX + CO_2 + HO_2 + NO_2$	KR02NO3*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	$HCOCOHC03 \rightarrow GLYOX + CO_2 + HO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G43428	TrGAroC	$METACETHO + OH \rightarrow CH_3C(O) + CO_2$	9.82E-11	Rickard and Pascoe (2009)
G43442	TrGAroCN	$HCOCOHPAN + OH \rightarrow GLYOX + CO + NO_2$	6.97E-11	Rickard and Pascoe (2009)
G43443	TrGAroCN	$HCOCOHPAN \rightarrow HCOCOHC03 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	$C_3_2OH_13CO + OH \rightarrow HCOCOHC03$	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	$HCOCOHC03H + OH \rightarrow HCOCOHC03$	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), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44001b	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$(k1_R02pR02*0.1273+k1_R02sR02*0.8727)*0.8727$	Rickard and Pascoe (2009), Sander et al. (2019)*
G44002	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N0}*(1-(0.1273*\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))) * 0.1273$	Rickard and Pascoe (2009), Sander et al. (2019)
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N0}*(1-(0.1273*\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))) * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2019)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*(0.1273*\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009)*
G44004a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	KR02N03*0.1273	Rickard and Pascoe (2009), Sander et al. (2019)
G44004b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	KR02N03*0.8727	Rickard and Pascoe (2009), Sander et al. (2019)
G44005a	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_s*f_{\text{tooh}}*f_{\text{alk}}*(k_p/(k_p+k_s))$	Sander et al. (2019)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_t*f_{\text{tooh}}*f_{\text{alk}}*(k_s/(k_p+k_s))$	Sander et al. (2019)
G44006a	TrGC	$i\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp}) * k_t / (3.*k_p+k_t)$	Atkinson (2003)
G44006b	TrGC	$i\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp}) * 3.*k_p / (3.*k_p+k_t)$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$k1_R02tR02$	Rickard and Pascoe (2009), Sander et al. (2019)
G44008	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{TC}_4\text{H}_9\text{OOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44009a	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02N0}*(1-\alpha_{\text{AN}}(4,3,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2019)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*\alpha_{\text{AN}}(4,3,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G44010a	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Sander et al. (2019)
G44010b	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$3.*k_p*f_{\text{tch2oh}}$	Sander et al. (2019)*
G44011	TrGCN	$\text{TC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$3.*k_p*f_{\text{ch2ono2}}$	Sander et al. (2019)*
G44012	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k1_R02sR02$	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44013	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$	$\text{KRO2H02}(4)$	Rickard and Pascoe (2009)
G44014a	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$	$\text{KRO2N0}*(1.-\text{alpha_AN}(4,2,0,0,0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2019)
G44014b	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC4H9NO3}$	$\text{KRO2N0}*\text{alpha_AN}(4,2,0,0,0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G44015a	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Sander et al. (2019)
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_s*f_sooh+2.*k_s+k_t*f_pch2oh$	Sander et al. (2019)*
G44016	TrGCN	$\text{IC4H9NO3} + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_s*f_ono2+2.*k_p+k_t*f_ch2ono2$	Sander et al. (2019)*
G44017	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .87 \text{MGLYOX} + .5481 \text{CO} + .1392 \text{HO}_2 + .1392 \text{OH} + .3219 \text{CH}_2\text{OO} + .13 \text{HCHO} + .04680 \text{OH} + .04680 \text{CO} + .07280 \text{CH}_3\text{C}(\text{O}) + .026 \text{CH}_3\text{CHO} + .026 \text{CO}_2 + .026 \text{HCHO} + .026 \text{HO}_2 + .02402 \text{MGLYOX} + .02402 \text{H}_2\text{O}_2 + .00718 \text{CH}_3\text{COCO}_2\text{H}$	$8.5\text{E}-16*\text{EXP}(-1520./\text{temp})$	Sander et al. (2019)
G44018	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{LHMVKABO2}$	$2.6\text{E}-12*\text{EXP}(610./\text{temp})$	Sander et al. (2019), Atkinson et al. (2006)*
G44019	TrGC	$\text{MEK} + \text{OH} \rightarrow \text{LMEKO2} + \text{H}_2\text{O}$	$1.5\text{E}-12*\text{EXP}(-90./\text{temp})$	Atkinson et al. (2006), Sander et al. (2019)*
G44020	TrGC	$\text{LMEKO2} + \text{HO}_2 \rightarrow \text{LMEKOOH}$	$\text{KRO2H02}(4)$	Sander et al. (2019)
G44021a	TrGCN	$\text{LMEKO2} + \text{NO} \rightarrow .62 \text{CH}_3\text{CHO} + .62 \text{CH}_3\text{C}(\text{O}) + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{KRO2N0}*(1.-(.62*\text{alpha_AN}(4,2,1,0,0, \text{temp}, \text{cair})+.38*\text{alpha_AN}(4,1,0,1,0, \text{temp}, \text{cair})))$	Sander et al. (2019)*
G44021b	TrGCN	$\text{LMEKO2} + \text{NO} \rightarrow \text{LMEKNO3}$	$\text{KRO2N0}*(.62*\text{alpha_AN}(4,2,1,0,0, \text{temp}, \text{cair})+.38*\text{alpha_AN}(4,1,0,1,0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44022a	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow \text{LMEKO2} + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Sander et al. (2019)
G44022b	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow .62 \text{BIACET} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O} + \text{OH}$	$(.62*k_t*f_tooh*f_co+.38*k_s*f_sooh)$	Sander et al. (2019)
G44023a	TrGCN	$\text{LC4H9NO3} + \text{OH} \rightarrow \text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_t*f_ono2*f_alk+k_p*f_alk+k_s*f_ch2ono2+k_p)*(k_s/(k_p+k_s))$	Sander et al. (2019)*
G44023b	TrGCN	$\text{LC4H9NO3} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_p+k_s*(1+f_ch2ono2+f_ono2)*f_alk)*(k_p/(k_p+k_s))$	Sander et al. (2019)*
G44024	TrGCN	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{NO}_2$	$3.2\text{E}-11$	Orlando et al. (2002)
G44025	TrGCN	$\text{MPAN} \rightarrow \text{MACO3} + \text{NO}_2$	k_PAN_M	see note*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44026	TrGC	LMEKO2 \rightarrow .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 \rightarrow .45 MACO3 + .55 MACRO2	8.E-12*EXP(380./temp)	Orlando et al. (1999b), Sander et al. (2019)
G44028	TrGC	MACR + O ₃ \rightarrow .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)	Sander et al. (2019)
G44029	TrGCN	MACR + NO ₃ \rightarrow MACO3 + HNO ₃	KN03AL*2.0	Rickard and Pascoe (2009)
G44030a	TrGC	MACO3 \rightarrow CH ₃ C(O) + HCHO + CO ₂	k1_R02RC03*0.9	Sander et al. (2019)
G44030b	TrGC	MACO3 \rightarrow MACO2H	k1_R02RC03*0.1	Sander et al. (2019)
G44031a	TrGC	MACO3 + HO ₂ \rightarrow MACO2 + OH	KAPH02*rc03_oh	Sander et al. (2019)
G44031b	TrGC	MACO3 + HO ₂ \rightarrow MACO3H	KAPH02*rc03_ooH	Sander et al. (2019)
G44031c	TrGC	MACO3 + HO ₂ \rightarrow MACO2H + O ₃	KAPH02*rc03_o3	Sander et al. (2019)
G44032	TrGCN	MACO3 + NO \rightarrow MACO2 + NO ₂	8.70E-12*EXP(290./temp)	Sander et al. (2019)
G44033	TrGCN	MACO3 + NO ₂ \rightarrow MPAN	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44034	TrGCN	MACO3 + NO ₃ \rightarrow MACO2 + NO ₂	KR02N03*1.60	Sander et al. (2019)
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	Sander et al. (2019)
G44036b	TrGC	MACRO2 + HO ₂ \rightarrow MACROOH	KR02H02(4)*rcoch2o2_ooH	Sander et al. (2019)
G44037a	TrGCN	MACRO2 + NO \rightarrow MACRO + NO ₂	KR02N0*(1.-alpha_AN(6,3,1,0,0, temp, cair))	Sander et al. (2019)
G44037b	TrGCN	MACRO2 + NO \rightarrow MACRN	KR02N0*alpha_AN(6,3,1,0,0,temp, cair)	Sander et al. (2019)
G44038	TrGCN	MACRO2 + NO ₃ \rightarrow MACRO + NO ₂	KR02N03	Sander et al. (2019)
G44039a	TrGC	MACROOH + OH \rightarrow MACRO2	0.6*k_CH300H_OH	Sander et al. (2019)
G44039b	TrGC	MACROOH + OH \rightarrow CO + CH ₃ COCH ₂ OH + OH	k_t*f_o*f_tch2oh*f_alk	Sander et al. (2019)
G44039c	TrGC	MACROOH + OH \rightarrow CO + MGLYOX + HO ₂	(k_s*f_soh*f_pch2oh + k_rohro)	Sander et al. (2019)
G44040	TrGC	MACROH + OH \rightarrow CH ₃ COCH ₂ OH + CO + HO ₂	k_t*f_o*f_tch2oh*f_alk	Sander et al. (2019)
G44041	TrGC	MACRO \rightarrow .885 CH ₃ COCH ₂ OH + .885 CO + .115 MGLYOX + .115 HCHO + HO ₂	KDEC	Sander et al. (2019)
G44042	TrGC	MACO2H + OH \rightarrow CH ₃ COCH ₂ OH + HO ₂ + CO ₂	((k_adt+k_adp)*a_co2h+k_co2h)	Sander et al. (2019)
G44043a	TrGC	MACO3H + OH \rightarrow CH ₃ COCH ₂ OH + CO ₂ + OH	(k_adt+k_adp)*a_co2h	Sander et al. (2019)
G44043b	TrGC	MACO3H + OH \rightarrow MACO3	0.6*k_CH300H_OH	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44044	TrGC	LHMVKABO2 → .024 CO2H3CHO + .072 MGLYOX + .072 HO2 + .072 HCHO + .5280 CH3C(O) + .5280 HOCH2CHO + .176 BIACETOH + .2 HO12CO3C4	(.12*k1_R02p0R02+.88*k1_R02s0R02)	Sander et al. (2019)
G44045a	TrGC	LHMVKABO2 + HO2 → OH + HOCH2CHO + CH3C(O)	KR02H02(4)*.88*rcoch2o2_oh	Sander et al. (2019)
G44045b	TrGC	LHMVKABO2 + HO2 → LHMVKABOOH	KR02H02(4)*(.12+.88*rcoch2o2_ooH)	Sander et al. (2019)
G44046a	TrGCN	LHMVKABO2 + NO → .12 MGLYOX + .12 HO2 + .88 HOCH2CHO + .88 CH3C(O) + .12 HCHO + NO2	KR02N0*(1-(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)))	Sander et al. (2019)
G44046b	TrGCN	LHMVKABO2 + NO → MVKNO3	KR02N0*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair))	Sander et al. (2019)*
G44047	TrGCN	LHMVKABO2 + NO3 → .12 MGLYOX + .12 HO2 + .88 HOCH2CHO + .88 CH3C(O) + .12 HCHO + .12 HO2 + NO2	KR02N03	Sander et al. (2019)
G44048a	TrGC	LHMVKABOOH + OH → LHMVKABO2	0.6*k_CH300H_OH	Sander et al. (2019)
G44048b	TrGC	LHMVKABOOH + OH → .12 CO2H3CHO + .88 BIACETOH + OH	(.12*k_s*f_sooH*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co)	Sander et al. (2019)
G44049a	TrGC	CO2H3CHO + OH → CO2H3CO3	k_t*f_o*f_alk	Sander et al. (2019)
G44049b	TrGC	CO2H3CHO + OH → CH3COCOCHO + HO2 + H2O	k_t*f_co*f_toh*f_cho	Sander et al. (2019)
G44050	TrGCN	CO2H3CHO + NO3 → CO2H3CO3 + HNO3	KN03AL*4.0	Rickard and Pascoe (2009)
G44051	TrGC	CO2H3CO3 → MGLYOX + HO2 + CO2	k1_R02RC03	Sander et al. (2019)
G44052a	TrGC	CO2H3CO3 + HO2 → OH + MGLYOX + HO2 + CO2	KAPH02*rc03_oh	Sander et al. (2019)
G44052b	TrGC	CO2H3CO3 + HO2 → CO2H3CO2H + O3	KAPH02*rc03_o3	Sander et al. (2019)
G44052c	TrGC	CO2H3CO3 + HO2 → CO2H3CO3H	KAPH02*rc03_ooH	Sander et al. (2019)
G44053	TrGCN	CO2H3CO3 + NO → MGLYOX + HO2 + NO2 + CO2	KAPNO	Sander et al. (2019)
G44054	TrGCN	CO2H3CO3 + NO3 → MGLYOX + HO2 + NO2 + CO2	KR02N03*1.60	Sander et al. (2019)
G44055a	TrGC	CO2H3CO3H + OH → CO2H3CO3	0.6*k_CH300H_OH	Sander et al. (2019)
G44055b	TrGC	CO2H3CO3H + OH → CH3C(O) + CO + CO2 + OH	(k_t*f_co2h*f_co*f_toh)	Sander et al. (2019)
G44056	TrGC	CO2H3CO2H + OH → CH3COCO2H + HO2	k_t*f_co2h*f_co*f_toh+k_co2h	Sander et al. (2019)
G44057a	TrGC	HO12CO3C4 + OH → BIACETOH + HO2	k_t*f_toh*f_alk*f_co	Sander et al. (2019)
G44057b	TrGC	HO12CO3C4 + OH → CO2H3CHO + HO2	k_s*f_soh*f_alk	Sander et al. (2019)
G44058	TrGC	MACO2 → .65 CH3 + .65 CO + .65 HCHO + .35 OH + .35 CH3COCH2O2 + CO2	KDEC	Sander et al. (2019)
G44059	TrGC	LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 CH3C(O) + OH	KHSD	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44060	TrGC	MACRO2 \rightarrow MGLYOX + HCHO + OH	KHSB	Sander et al. (2019)
G44061a	TrGCN	MVKNO3 + OH \rightarrow MGLYOX + CO ₂ + HO ₂ + NO ₂ + H ₂ O	k_s*f_sooh*f_ch2ono2+k_rohro	Sander et al. (2019)*
G44061b	TrGCN	MVKNO3 + OH \rightarrow BIACETOH + NO ₂ + H ₂ O	k_t*f_ono2*f_co*f_pch2oh	Sander et al. (2019)*
G44062a	TrGCN	MACRN + OH \rightarrow CH ₃ COCH ₂ OH + CO ₂ + NO ₂ + H ₂ O	k_t*f_o*f_ch2ono2	Sander et al. (2019)*
G44062b	TrGCN	MACRN + OH \rightarrow MGLYOX + CO + NO ₂ + H ₂ O	k_rohro+k_s*f_sooh*f_ch2ono2	Sander et al. (2019)*
G44063	TrGC	MACRO2 \rightarrow CH ₃ COCH ₂ OH + OH + CO	K14HSAL	Sander et al. (2019)
G44064	TrGC	EZCH3CO2CHCHO \rightarrow .9 CH ₃ COCHCO + .1 CH ₃ C(O) + .01 GLYOX + .18 CO + .09 HO ₂ + OH	K15HS24VYNAL	Sander et al. (2019)
G44065	TrGC	EZCH3CO2CHCHO + HO ₂ \rightarrow CH ₃ COOHCHCHO	KR02H02(4)	Sander et al. (2019)
G44066	TrGCN	EZCH3CO2CHCHO + NO \rightarrow CH ₃ COCHO ₂ CHO + NO ₂	KR02N0	Sander et al. (2019)*
G44067	TrGCN	EZCH3CO2CHCHO + NO ₃ \rightarrow CH ₃ COCHO ₂ CHO + NO ₂	kR02N03	Sander et al. (2019)
G44068	TrGC	EZCH3CO2CHCHO \rightarrow CH ₃ COCHO ₂ CHO	k1_R02sOR02	Sander et al. (2019)
G44069	TrGC	EZCHOCCH3CHO2 \rightarrow HCOCCH ₃ CO + OH	K15HS24VYNAL	Sander et al. (2019)
G44070	TrGCN	EZCHOCCH3CHO2 + NO \rightarrow HCOCO ₂ CH ₃ CHO + NO ₂	KR02N0	Sander et al. (2019)*
G44071	TrGC	EZCHOCCH3CHO2 + HO ₂ \rightarrow HCOCCH ₃ CHOOH	KR02H02(4)	Sander et al. (2019)
G44072	TrGCN	EZCHOCCH3CHO2 + NO ₃ \rightarrow HCOCO ₂ CH ₃ CHO + NO ₂	KR02N03	Sander et al. (2019)
G44073	TrGC	EZCHOCCH3CHO2 \rightarrow HCOCO ₂ CH ₃ CHO	k1_R02pOR02	Sander et al. (2019)
G44074	TrGC	CH ₃ COOHCHCHO \rightarrow CH ₃ COCHO ₂ CHO + OH	KHYDEC	Sander et al. (2019)
G44075	TrGC	HCOCCH ₃ CHOOH \rightarrow HCOCO ₂ CH ₃ CHO + OH	KHYDEC	Sander et al. (2019)
G44076	TrGCN	CH ₃ COCHO ₂ CHO + NO \rightarrow CH ₃ C(O) + GLYOX + NO ₂	KR02N0	Sander et al. (2019)*
G44077	TrGCN	CH ₃ COCHO ₂ CHO + NO ₃ \rightarrow CH ₃ C(O) + GLYOX + NO ₂	KR02N03	Sander et al. (2019)
G44078	TrGC	CH ₃ COCHO ₂ CHO + HO ₂ \rightarrow CH ₃ C(O) + GLYOX + OH	KR02H02(4)	Sander et al. (2019)*
G44079	TrGC	CH ₃ COCHO ₂ CHO \rightarrow CH ₃ C(O) + GLYOX	k1_R02sOR02	Sander et al. (2019)
G44080	TrGC	HCOCO ₂ CH ₃ CHO \rightarrow MGLYOX + CO + HO ₂	k1_R02tOR02	Sander et al. (2019)
G44081	TrGCN	HCOCO ₂ CH ₃ CHO + NO \rightarrow MGLYOX + CO + HO ₂ + NO ₂	KR02N0	Sander et al. (2019)*
G44082	TrGC	HCOCO ₂ CH ₃ CHO + HO ₂ \rightarrow MGLYOX + CO + HO ₂ + OH	KR02H02(4)	Sander et al. (2019)*
G44083	TrGCN	HCOCO ₂ CH ₃ CHO + NO ₃ \rightarrow MGLYOX + CO + HO ₂ + NO ₂	KR02N03	Sander et al. (2019)
G44084	TrGC	HCOCCH ₃ CO + OH \rightarrow CO + MGLYOX + HO ₂	1E-10*a_cho	Hatakeyama et al. (1985), Sander et al. (2019)
G44085	TrGC	CH ₃ COCHCO + OH \rightarrow CO + MGLYOX + HO ₂	7.6E-11*a_coch3	Hatakeyama et al. (1985), Sander et al. (2019)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44086	TrGCN	LMEKNO3 + OH → .62 MGLYOX + .62 HCHO + .62 HO ₂ + .62 NO ₂ + .38 CH ₃ C(O) + .38 NO ₃ CH ₂ CHO	.62*(k_p*(f_co+f_ch2ono2)) + .38*(k_s*f_ch2ono2*f_co)	Sander et al. (2019)*
G44087	TrGC	MEPROPENE + OH → IBUTOLBO2	9.4E-12*EXP(505./temp)	Atkinson et al. (2006)
G44088a	TrGC	MEPROPENE + O ₃ → CH ₃ COCH ₃ + CH ₂ OO*	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Sander et al. (2019)
G44088b	TrGC	MEPROPENE + O ₃ → CH ₃ COCH ₂ O ₂ + OH + HCHO	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Sander et al. (2019)
G44089	TrGCN	MEPROPENE + NO ₃ → CH ₃ COCH ₃ + HCHO + NO ₂	3.4E-13	Atkinson et al. (2006), Sander et al. (2019)*
G44090	TrGC	IBUTOLBO2 → CH ₃ COCH ₃ + HCHO + HO ₂	k1_R02tOR02	Sander et al. (2019)
G44091a	TrGC	IBUTOLBO2 + HO ₂ → IBUTOLBOOH	KR02H02(4)*rcoch2o2_ooh	Sander et al. (2019)
G44091b	TrGC	IBUTOLBO2 + HO ₂ → CH ₃ COCH ₃ + HCHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Sander et al. (2019)
G44092a	TrGCN	IBUTOLBO2 + NO → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(5,3,0,0,0,temp, cair))	Sander et al. (2019)
G44092b	TrGCN	IBUTOLBO2 + NO → IBUTOLBNO3	KR02N0*alpha_AN(5,3,0,0,0,temp, cair)	Sander et al. (2019)
G44093	TrGCN	IBUTOLBO2 + NO ₃ → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02N03	Sander et al. (2019)
G44094a	TrGC	IBUTOLBOOH + OH → IBUTOLBO2	.6*k_CH300H_OH	Sander et al. (2019)
G44094b	TrGC	IBUTOLBOOH + OH → CH ₃ COCH ₃ + HCHO + HO ₂	k_s*f_sooh*f_pch2oh	Sander et al. (2019)
G44095	TrGCN	IBUTOLBNO3 + OH → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	3.*k_p	Sander et al. (2019)
G44096	TrGC	BUT1ENE + OH → LBUT1ENO2	6.6E-12*EXP(465./temp)	Atkinson et al. (2006)*
G44097a	TrGC	BUT1ENE + O ₃ → HCHO + .5 C ₂ H ₅ CHO + .5 H ₂ O ₂ + .5 CH ₃ CHO + .5 CO + .5 HO ₂	3.35E-15*EXP(-1745./temp)*.57	Atkinson et al. (2006), Sander et al. (2019)*
G44097b	TrGC	BUT1ENE + O ₃ → C ₂ H ₅ CHO + CH ₂ OO*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Sander et al. (2019)*
G44098	TrGCN	BUT1ENE + NO ₃ → C ₂ H ₅ CHO + HCHO + NO ₂	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44099	TrGC	LBUT1ENO2 → C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02sOR02	Sander et al. (2019)
G44100a	TrGC	LBUT1ENO2 + HO ₂ → LBUT1ENOOH	KR02H02(4)*rcoch2o2_ooh	Sander et al. (2019)
G44100b	TrGC	LBUT1ENO2 + HO ₂ → C ₂ H ₅ CHO + HCHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44101a	TrGCN	$\text{LBUT1ENO2} + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\text{alpha_AN}(5,2,0,0,0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44101b	TrGCN	$\text{LBUT1ENO2} + \text{NO} \rightarrow \text{LBUT1ENNO3}$	$\text{KR02N0}*\text{alpha_AN}(5,2,0,0,0, \text{temp}, \text{cair})$	Sander et al. (2019)
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	Sander et al. (2019)
G44103a	TrGC	$\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{LBUT1ENO2}$.6*k_CH300H_OH	Sander et al. (2019)
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	Sander et al. (2019)*
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	Sander et al. (2019)*
G44105	TrGC	$\text{CBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$	$1.1\text{E-}11*\text{EXP}(485./\text{temp})$	Atkinson et al. (2006)
G44106	TrGC	$\text{CBUT2ENE} + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + .16 \text{CH}_3\text{CHOHOOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	$3.2\text{E-}15*\text{EXP}(-965./\text{temp})$	Atkinson et al. (2006), Sander et al. (2019)*
G44107	TrGCN	$\text{CBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{CH}_3\text{CHO} + \text{NO}_2$	3.5E-13	Atkinson et al. (2006), Sander et al. (2019)*
G44108	TrGC	$\text{TBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$	$1.0\text{E-}11*\text{EXP}(553./\text{temp})$	Atkinson et al. (2006)
G44109	TrGC	$\text{TBUT2ENE} + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + .16 \text{CH}_3\text{CHOHOOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	$6.6\text{E-}15*\text{EXP}(-1060./\text{temp})$	Atkinson et al. (2006), Sander et al. (2019)
G44110	TrGCN	$\text{TBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{CH}_3\text{CHO} + \text{NO}_2$	$1.78\text{E-}12*\text{EXP}(-530./\text{temp}) + 1.28\text{E-}14*\text{EXP}(570./\text{temp})$	Atkinson et al. (2006), Sander et al. (2019)*
G44111	TrGC	$\text{BUT2OLO2} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2$	k1_R02sOR02	Sander et al. (2019)
G44112a	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow \text{BUT2OLOOH}$	$\text{KR02H02}(4)*\text{rcoch2o2_ooh}$	Sander et al. (2019)
G44112b	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(4)*\text{rcoch2o2_oh}$	Sander et al. (2019)
G44113a	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\text{alpha_AN}(5,2,0,0,0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44113b	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow \text{BUT2OLNO3}$	$\text{KR02N0}*\text{alpha_AN}(5,2,0,0,0, \text{temp}, \text{cair})$	Sander et al. (2019)
G44114	TrGCN	$\text{BUT2OLO2} + \text{NO}_3 \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44115a	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO2}$.6*k_CH300H_OH	Sander et al. (2019)
G44115b	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{LMEKOOH} + \text{HO}_2$	k_t*f_toh*f_pch2oh	Sander et al. (2019)
G44115c	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO} + \text{OH}$	k_t*f_tooh*f_pch2oh	Sander et al. (2019)
G44116	TrGCN	$\text{BUT2OLNO3} + \text{OH} \rightarrow \text{LMEKNO3} + \text{HO}_2$	k_t*f_toh*f_ch2ono2	Sander et al. (2019)
G44117	TrGC	$\text{BUT2OLO} + \text{OH} \rightarrow \text{BIACET} + \text{HO}_2$	k_t*f_toh*f_co	Sander et al. (2019)
G44118	TrGC	$\text{IPRCHO} + \text{OH} \rightarrow \text{IPRCO3} + \text{H}_2\text{O}$	$6.8\text{E-}12*\text{EXP}(410./\text{temp})$	Atkinson et al. (2006)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44119	TrGCN	$\text{IPRCHO} + \text{NO}_3 \rightarrow \text{IPRCO}_3 + \text{HNO}_3$	$1.67\text{E}-12 * \text{EXP}(-1460./\text{temp})$	Atkinson et al. (2006)
G44120	TrGC	$\text{IPRCO}_3 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)
G44121a	TrGC	$\text{IPRCO}_3 + \text{HO}_2 \rightarrow \text{PERIBUACID}$	KAPH02*rc03_ooh	Rickard and Pascoe (2009), Sander et al. (2019)
G44121b	TrGC	$\text{IPRCO}_3 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*(1-rc03_ooh)	Rickard and Pascoe (2009), Sander et al. (2019)
G44122	TrGCN	$\text{IPRCO}_3 + \text{NO}_2 \rightarrow \text{PIP}_N$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44123	TrGCN	$\text{IPRCO}_3 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G44124a	TrGC	$\text{PERIBUACID} + \text{OH} \rightarrow \text{IPRCO}_3 + \text{H}_2\text{O}$.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44124b	TrGC	$\text{PERIBUACID} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{CO}_2$	k_s*f_co2h	Sander et al. (2019)*
G44125	TrGCN	$\text{PIP}_N \rightarrow \text{IPRCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	$\text{PIP}_N + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{NO}_2$	k_s*f_cpan	Sander et al. (2019)*
G44127	TrGC	$\text{MPROPENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{COCH}_3$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G44128	TrGC	$\text{MPROPENOL} + \text{HCOOH} \rightarrow \text{IPRCHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44129	TrGC	$\text{IPRCHO} + \text{HCOOH} \rightarrow \text{MPROPENOL} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44130	TrGC	$\text{BUTENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C}_2\text{H}_5\text{CHO}$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G44131	TrGC	$\text{BUTENOL} + \text{HCOOH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44132	TrGC	$\text{C}_3\text{H}_7\text{CHO} + \text{HCOOH} \rightarrow \text{BUTENOL} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44133	TrGC	$\text{HVMK} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	$\text{HVMK} + \text{HCOOH} \rightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44135	TrGC	$\text{CO}_2\text{C}_3\text{CHO} + \text{HCOOH} \rightarrow \text{HVMK} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44136	TrGC	$\text{HMAC} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	$\text{HMAC} + \text{HCOOH} \rightarrow \text{IBUTDIAL} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44138	TrGC	IBUTDIAL + HCOOH → HMAC + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44139	TrGC	CO2C3CHO + OH → CH ₃ COCH ₂ O ₂ + CO ₂ + H ₂ O	k_t*f_o*f_alk+k_s*f_cho*f_co	Sander et al. (2019)*
G44140	TrGCN	CO2C3CHO + NO ₃ → CH ₃ COCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*4.0	Sander et al. (2019)*
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	Sander et al. (2019)*
G44142	TrGCN	IBUTDIAL + NO ₃ → CH ₃ CHO + CO + HO ₂ + CO ₂ + HNO ₃	2.*KN03AL*4.0	Sander et al. (2019)*
G44200	TrGTerC	CH ₃ COCOCH ₂ O ₂ → CH ₃ C(O) + HCHO + CO	k1_R02pOR02	Rickard and Pascoe (2009)
G44201	TrGTerC	CH ₃ COCOCH ₂ O ₂ + HO ₂ → CH ₃ COCOCH ₂ OOH	KR02H02(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	C44O2 + HO ₂ → C44OOH	KR02H02(4)	Rickard and Pascoe (2009)
G44205	TrGTerCN	C44O2 + NO → HCOCH ₂ CHO + CO ₂ + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O2 → HCOCH ₂ CHO + CO ₂ + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)
G44207	TrGTerC	C44OOH + OH → C44O2	7.46E-11	Rickard and Pascoe (2009)
G44208	TrGTerC	CHOC3COO2 → HCOCH ₂ CO3 + HCHO	k1_R02pOR02	Rickard and Pascoe (2009)
G44209	TrGTerC	CHOC3COO2 + HO ₂ → C413COOOH	KR02H02(4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	CHOC3COO2 + NO → HCOCH ₂ CO3 + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44211	TrGTerC	C413COOOH + OH → CHOC3COO2	8.33E-11	Rickard and Pascoe (2009)
G44212	TrGTerC	C4CODIAL + OH → C312COCO3	3.39E-11	Rickard and Pascoe (2009)
G44213	TrGTerCN	C4CODIAL + NO ₃ → C312COCO3 + HNO ₃	2.*KN03AL*4.0	Rickard and Pascoe (2009)
G44214	TrGTerC	C312COCO3 → HCOCOCH ₂ O ₂ + CO ₂	k1_R02RCO3	Rickard and Pascoe (2009)
G44215a	TrGTerC	C312COCO3 + HO ₂ → C312COCO3H	KAPH02*rco3_ooH	Rickard and Pascoe (2009)
G44215b	TrGTerC	C312COCO3 + HO ₂ → HCOCOCH ₂ O ₂ + CO ₂ + OH	KAPH02*(1-rco3_ooH)	Rickard and Pascoe (2009)
G44216	TrGTerCN	C312COCO3 + NO ₂ → C312COPAN	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44217	TrGTerCN	C312COCO3 + NO → HCOCOCH ₂ O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44218	TrGTerC	C312COCO3H + OH → C312COCO3	1.63E-11	Rickard and Pascoe (2009)
G44219	TrGTerCN	C312COPAN → C312COCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44220	TrGTerCN	C312COPAN + OH → HCOCOCHO + CO + NO ₂	1.27E-11	Rickard and Pascoe (2009)
G44221	TrGTerC	CH ₃ COCOCHO + OH → CH ₃ C(O) + 2 CO	8.4E-13*EXP(830./temp)	Sander et al. (2019)*
G44222	TrGTerCN	CH ₃ COCOCHO + NO ₃ → CH ₃ C(O) + 2 CO + HNO ₃	KN03AL*4.0	Rickard and Pascoe (2009)
G44223	TrGTerC	IBUTALOH + OH → IPRHOCO3	1.4E-11	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44224a	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*rc03_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G44224b	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO2H} + \text{O}_3$	KAPH02*rc03_o3	Rickard and Pascoe (2009), Sander et al. (2019)
G44224c	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO3H}$	KAPH02*rc03_ooh	Rickard and Pascoe (2009), Sander et al. (2019)
G44225	TrGTerCN	$\text{IPRHOCO3} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G44226	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_2 \rightarrow \text{C4PAN5}$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44227	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G44228a	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.7	Rickard and Pascoe (2009)
G44228b	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{IPRHOCO2H}$	k1_R02RC03*0.3	Rickard and Pascoe (2009)
G44229	TrGTerC	$\text{IPRHOCO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	1.72E-12	Rickard and Pascoe (2009)
G44230	TrGTerC	$\text{OH} + \text{IPRHOCO3H} \rightarrow \text{IPRHOCO3}$	4.80E-12	Rickard and Pascoe (2009)
G44231	TrGTerCN	$\text{C4PAN5} \rightarrow \text{IPRHOCO3} + \text{NO}_2$	K_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	$\text{C4PAN5} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO} + \text{NO}_2$	4.75E-13	Rickard and Pascoe (2009)
G44233a	TrGTerC	$\text{MBOOO} \rightarrow \text{IPRHOCO2H}$	1.60E-17*C(ind_H20)*(0.08+0.15)	Rickard and Pascoe (2009), Sander et al. (2019)
G44233b	TrGTerC	$\text{MBOOO} \rightarrow \text{IBUTALOH} + \text{H}_2\text{O}_2$	1.60E-17*C(ind_H20)*0.77	Rickard and Pascoe (2009), Sander et al. (2019)
G44234	TrGTerC	$\text{MBOOO} + \text{CO} \rightarrow \text{IBUTALOH} + \text{CO}_2$	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	$\text{MBOOO} + \text{NO} \rightarrow \text{IBUTALOH} + \text{NO}_2$	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	$\text{MBOOO} + \text{NO}_2 \rightarrow \text{IBUTALOH} + \text{NO}_3$	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	$\text{MALANHY} + \text{OH} \rightarrow \text{MALANHYO2}$	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{HOCOC4DIAL} + \text{OH}$	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{MALDIALO2}$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44402	TrGAroCN	$\text{NC4DCO2H} + \text{OH} \rightarrow \text{MALANHY} + \text{NO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G44403	TrGAroC	$\text{CO14O3CO2H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + 2 \text{CO}_2$	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	$\text{BZFUOOH} + \text{OH} \rightarrow \text{BZFUO2}$	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	$\text{HOCOC4DIAL} + \text{OH} \rightarrow \text{CO2C4DIAL} + \text{HO}_2$	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow \text{MALDALCO2H} + \text{O}_3$	KAPH02*rc03_o3	Rickard and Pascoe (2009)
G44406b	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow \text{MALDALCO3H}$	KAPH02*rc03_ooh	Rickard and Pascoe (2009)
G44406c	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2 + \text{OH}$	KAPH02*rc03_oh	Rickard and Pascoe (2009)*
G44407	TrGAroCN	$\text{MALDIALCO3} + \text{NO} \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44408	TrGAroCN	MALDIALCO3 + NO ₂ → MALDIALPAN	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO3 + NO ₃ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)*
G44410	TrGAroC	MALDIALCO3 → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO ₃ → NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O ₃ → .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H ₂ O ₂ + .5 CO + .5 CO ₂ + .5 HCOCH ₂ O ₂ + .5 OH	2.20E-19	see note*
G44413	TrGAroC	BZFUONE + OH → BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH → NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH → MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH → C3DIALO2 + CO ₂	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO ₂ → C3DIALO2 + CO ₂ + OH	KAPH02*rc03_oh	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO ₂ → EPXDLCO2H + O ₃	KAPH02*rc03_o3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO ₂ → EPXDLCO3H	KAPH02*rc03_ooH	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO → C3DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44419	TrGAroCN	EPXDLCO3 + NO ₂ → EPXDLPAN	k_CH3C03_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*KNO3AL*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-rc0ch2o2_ oh-rch0ch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2019)
G44429b	TrGAroC	MALANHYO2 + HO ₂ → HCOCOHC03 + CO ₂ + OH	KR02H02(4)*(rc0ch2o2_oh+ rch0ch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2019)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCOHC03 + CO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G44431	TrGAroCN	MALANHYO2 + NO ₃ → HCOCOHCOC3 + CO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 → HCOCOHCOC3 + 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), Sander et al. (2019)
G44435b	TrGAroCN	NBZFUO2 + HO ₂ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G44436	TrGAroCN	NBZFUO2 + NO → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂	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)
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), Sander et al. (2019)
G44442b	TrGAroC	MECOACETO2 + HO ₂ → CH ₃ C(O)OO + HCHO + CO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
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), Sander et al. (2019)
G44449b	TrGAroC	BZFUO2 + HO ₂ → CO14O3CHO + HO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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_R02sOR02	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_R02sOR02	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH → HCOCOCHO + CO + NO ₂	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN → EPXDLCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH → MECOACETO2	3.59E-12	Rickard and Pascoe (2009)
G45000	TrGC	C ₅ H ₈ + O ₃ → .3508 MACR + .01518 MACO2H + .2440 MVK + .7085 HCHO + .11 CH ₂ OO + .1275 C ₃ H ₆ + .1575 CH ₃ C(O) + .0510 CH ₃ + .2625 HO ₂ + .27 OH + .09482 H ₂ O ₂ + .255 CO ₂ + .522 CO + .07182 HCHO + .03618 HCOCH ₂ O ₂ + .01782 CO + 0.05408 LCARBON	1.03E-14*EXP(-1995./temp)	Atkinson et al. (2006), Sander et al. (2019)
G45001	TrGC	C ₅ H ₈ + OH → .63 ISOPAB + .30 ISOPCD + .07 LISOPEFO2	2.7E-11*EXP(390./temp)	Atkinson et al. (2006), Sander et al. (2019)
G45002	TrGCN	C ₅ H ₈ + NO ₃ → NISOPO2	3.0E-12*EXP(-450./temp)	Atkinson et al. (2006)
G45003a	TrGC	ISOPAB + O ₂ → LISOPACO2	5.530E-13	Sander et al. (2019)
G45003b	TrGC	ISOPAB + O ₂ → ISOPBO2	3.E-12	Sander et al. (2019)
G45004a	TrGC	ISOPCD + O ₂ → LDISOPACO2	6.780E-13	Sander et al. (2019)
G45004b	TrGC	ISOPCD + O ₂ → ISOPDO2	3.E-12	Sander et al. (2019)
G45005	TrGC	LISOPACO2 → ISOPAB + O ₂	3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4	Sander et al. (2019)
G45006	TrGC	ISOPBO2 → ISOPAB + O ₂	3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp)	Sander et al. (2019)
G45007	TrGC	LDISOPACO2 → ISOPCD + O ₂	5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58	Sander et al. (2019)
G45008	TrGC	ISOPDO2 → ISOPCD + O ₂	5.0E14*exp(-10120./temp)+8.25E14*exp(-10220./temp)	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45009a	TrGC	LISOPACO2 → C1ODC2O2C4OOH	K16HSZ14 * 2./3.*(1-fhpal)	Sander et al. (2019)
G45009b	TrGC	LISOPACO2 → ZCODC23DBCOOH + HO ₂	K16HSZ14 * (2./3.*fhpal + 1./3.)	Sander et al. (2019)
G45010a	TrGC	LDISOPACO2 → C1OOHC3O2C4OD	k16HSZ41 * 2./3.*(1-fhpal)	Sander et al. (2019)
G45010b	TrGC	LDISOPACO2 → ZCODC23DBCOOH + HO ₂	k16HSZ41 * (2./3.*fhpal + 1./3.)	Sander et al. (2019)
G45011	TrGC	LISOPACO2 → .9 LISOPACO + .1 ISOPA0H	k1_R02LISOPACO2	Rickard and Pascoe (2009), Sander et al. (2019)
G45012	TrGC	LISOPACO2 + HO ₂ → LISOPACOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45013a	TrGCN	LISOPACO2 + NO → LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45013b	TrGCN	LISOPACO2 + NO → LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0, temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45014	TrGCN	LISOPACO2 + NO ₃ → LISOPACO + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45015	TrGC	LDISOPACO2 → .9 LISOPACO + .1 ISOPA0H	k1_R02LISOPACO2	Rickard and Pascoe (2009), Sander et al. (2019)
G45016	TrGC	LDISOPACO2 + HO ₂ → LISOPACOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO → LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45017b	TrGCN	LDISOPACO2 + NO → LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0, temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45018	TrGCN	LDISOPACO2 + NO ₃ → LISOPACO + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH → LISOPACO2	0.6*k_CH300H_OH	Sander et al. (2019)
G45019b	TrGC	LISOPACOOH + OH → ZCODC23DBCOOH + HO ₂	k_s*f_allyl*f_soh	Sander et al. (2019)
G45019c	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH	(k_s*f_soh*f_allyl+ k_rohro)	Sander et al. (2019)
G45019d	TrGC	LISOPACOOH + OH → LIEPOX + OH	(k_adt+k_ads)*a_ch2oh*a_ch2ooh	Sander et al. (2019)*
G45020	TrGC	ISOPA0H + OH → LHC4ACCHO + HO ₂	(k_adt+k_ads)*a_ch2oh*a_ch2oh+k_s*f_soh*f_allyl+k_rohro	Sander et al. (2019)
G45021	TrGCN	LISOPACNO3 + OH → LISOPACNO3O2	(k_adt+k_ads)*a_ch2ono2*a_ch2oh	Sander et al. (2019)*
G45022	TrGC	ISOPBO2 → .8 MVK + .8 HCHO + .8 HO ₂ + .2 ISOPBOH	k1_R02ISOPBO2	Rickard and Pascoe (2009)
G45023a	TrGC	ISOPBO2 + HO ₂ → ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2019)
G45023b	TrGC	ISOPBO2 + HO ₂ → MVK + HCHO + HO ₂ + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45024a	TrGCN	ISOPBO2 + NO → MVK + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(6,3,0,0,0, temp, cair))	Lockwood et al. (2010), Sander et al. (2019)
G45024b	TrGCN	ISOPBO2 + NO → ISOPBNO3	KR02N0*alpha_AN(6,3,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45025	TrGCN	ISOPBO2 + NO ₃ → MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45026a	TrGC	ISOPBOOH + OH → LIEPOX + OH	(k_ads+k_adp)*a_ch2ooh	Paulot et al. (2009b), Sander et al. (2019)
G45026b	TrGC	ISOPBOOH + OH → ISOPBO2	0.6*k_CH300H_OH	Sander et al. (2019)
G45026c	TrGC	ISOPBOOH + OH → MGLYOX + HOCH ₂ CHO	k_rohro+k_s*f_alk*f_soh	Sander et al. (2019)
G45027	TrGC	ISOPBOOH + O ₃ → .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	Sander et al. (2019)
G45028	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃	k_s*f_alk*f_soh+(k_adp+k_ads)*a_ch2oh	Sander et al. (2019)
G45029	TrGCN	ISOPBNO3 + OH → ISOPBDNO3O2	(k_adt+k_adp)*f_ch2ono2	Sander et al. (2019)
G45030	TrGC	ISOPDO2 → .8 MACR + .8 HCHO + .8 HO ₂ + .1 HCOC5 + .1 ISOPDOH	k1_R02ISOPD02	Rickard and Pascoe (2009)
G45031a	TrGC	ISOPDO2 + HO ₂ → ISOPDOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2019)
G45031b	TrGC	ISOPDO2 + HO ₂ → MACR + HCHO + HO ₂ + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2019)
G45032a	TrGCN	ISOPDO2 + NO → MACR + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(6,2,0,0,0, temp, cair))	Lockwood et al. (2010), Sander et al. (2019)
G45032b	TrGCN	ISOPDO2 + NO → ISOPDNO3	KR02N0*alpha_AN(6,2,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45033	TrGCN	ISOPDO2 + NO ₃ → MACR + HCHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45034a	TrGC	ISOPDOOH + OH → LIEPOX + OH	(k_adt+k_adp)*a_ch2ooh	Paulot et al. (2009b), Sander et al. (2019)
G45034b	TrGC	ISOPDOOH + OH → ISOPDO2	0.6*k_CH300H_OH	Sander et al. (2019)
G45034c	TrGC	ISOPDOOH + OH → HCOC5 + OH	k_t*f_tooh*f_allyl*f_pch2oh	Sander et al. (2019)
G45034d	TrGC	ISOPDOOH + OH → CH ₃ COCH ₂ OH + GLYOX + OH	k_s*f_pch2oh*f_soh	Sander et al. (2019)
G45035	TrGC	ISOPDOOH + O ₃ → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO ₂ + .2079 CO + .1221 CH ₂ OO	1.E-17	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45036	TrGC	ISOPDOH + OH → HCOC5 + HO ₂	2.*k_rohro+(k_t*f_toh*f_allyl+k_s*f_soh)*f_pch2oh+(k_adt+k_adp)*a_ch2oh	Sander et al. (2019)
G45037	TrGCN	ISOPDNO3 + OH → ISOPBDNO3O2	(k_adp+k_ads)*a_ch2ono2	Sander et al. (2019)*
G45038	TrGCN	NISOP02 → .8 NC4CHO + .6 HO ₂ + .2 LISOPACNO3	k1_R02LISOPAC02	Rickard and Pascoe (2009)
G45039	TrGCN	NISOP02 + HO ₂ → NISOP0OH	KR02H02(5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOP02 + NO → NC4CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOP02 + NO ₃ → NC4CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45042	TrGCN	NISOP0OH + OH → NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC4CHO + OH → LNISO3	(k_adt+k_ads)*a_cho*a_ch2ono2	Sander et al. (2019)*
G45044	TrGCN	NC4CHO + O ₃ → .27 NOA + .027 HCOCO 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	Sander et al. (2019)
G45045	TrGCN	NC4CHO + NO ₃ → LNISO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO3 + HO ₂ → LNISOOH	.5*KR02H02(5) + .5*KAPH02	Rickard and Pascoe (2009)
G45047	TrGCN	LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	.5*KAPNO +.5*KR02N0	Rickard and Pascoe (2009)*
G45048	TrGCN	LNISO3 + NO ₃ → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	1.3*KR02N03	Rickard and Pascoe (2009)
G45049	TrGCN	LNISOOH + OH → LNISO3	2.65E-11	Rickard and Pascoe (2009)
G45050a	TrGC	LHC4ACCHO + OH → LC578O2	(k_adtertprim+k_ads)*a_cho*a_ch2oh	Sander et al. (2019)
G45050b	TrGC	LHC4ACCHO + OH → LHC4ACCO3	k_t*f_o	Sander et al. (2019)
G45050c	TrGC	LHC4ACCHO + OH → C4MDIAL + HO ₂	k_s*f_soh*f_allyl	Sander et al. (2019)
G45051	TrGC	LHC4ACCHO + O ₃ → .2225 CH 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_ooH	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45055	TrGCN	$\text{LC578O2} + \text{NO} \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45056	TrGCN	$\text{LC578O2} + \text{NO}_3 \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45057	TrGC	$\text{LC578O2} \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCH}_2\text{CHO} + .75 \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	KHSB	Sander et al. (2019)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	$0.6 * k_{\text{CH300H_OH}}$	Sander et al. (2019)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C10DC2OOHC4OD} + \text{HO}_2$	$k_{\text{t*o*f_tch2oh*f_alk+k_t*f_toh*f_pch2oh*f_pch2oh+k_s*f_soh*f_pch2oh}}$	Sander et al. (2019)
G45059a	TrGC	$\text{LHC4ACCO3} \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMVKABO2} + \text{CO}_2$	$k1_{\text{R02RC03}} * 0.9$	Sander et al. (2019)
G45059b	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LHC4ACCO2H}$	$k1_{\text{R02RC03}} * 0.1$	Sander et al. (2019)
G45060a	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 2 \text{OH} + .5 \text{MACRO2} + .5 \text{LHMVKABO2} + \text{CO}_2$	KAPH02*rc03_oh	Sander et al. (2019)
G45060b	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO3H}$	KAPH02*rc03_ooh	Sander et al. (2019)
G45060c	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$	KAPH02*rc03_o3	Sander et al. (2019)
G45061	TrGCN	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{MACRO2} + .5 \text{LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KAPN0	Sander et al. (2019)
G45062	TrGCN	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G45063	TrGCN	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{MACRO2} + .5 \text{LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	$1.6 * \text{KR02N03}$	Sander et al. (2019)
G45064a	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMVKABO2} + \text{CO}_2$	$2.52\text{E-}11$	Sander et al. (2019)
G45064b	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$2.88\text{E-}11$	Rickard and Pascoe (2009)
G45065	TrGCN	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G45066	TrGCN	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{MACROH} + .5 \text{HO12CO3C4} + \text{CO} + \text{NO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)
G45067	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	$3.81\text{E-}11$	Rickard and Pascoe (2009)
G45068	TrGC	$\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{H}_2\text{O}_2 + .67 \text{HCHO} + .2079 \text{CO} + .1221 \text{CH}_2\text{OO} + .05280 \text{OH}$	$7.51\text{E-}16 * \text{EXP}(-1521./\text{temp})$	Sander et al. (2019)
G45069	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH2CO}$	$k1_{\text{R02tOR02}}$	Sander et al. (2019)
G45070a	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH2CO}$	$\text{KR02H02(5)*rcoch2o2_oh}$	Sander et al. (2019)
G45070b	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	$\text{KR02H02(5)*rcoch2o2_ooh}$	Sander et al. (2019)
G45071	TrGCN	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH2CO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45072	TrGCN	$C59O2 + NO_3 \rightarrow CH_3COCH_2OH + HOCH_2CO + NO_2$	KR02N03	Sander et al. (2019)
G45073	TrGC	$C59OOH + OH \rightarrow C59O2$	9.7E-12	Rickard and Pascoe (2009)
G45074	TrGC	$LIEPOX + OH \rightarrow DB1O2 + H_2O$	$5.78E-11 * EXP(-400./temp) * (1.52/3.+0.98*2./3.)/1.51$	Paulot et al. (2009b), Bates et al. (2014), Sander et al. (2019)*
G45075	TrGC	$ISOPBO2 \rightarrow MVK + HCHO + OH$	KHSB	Sander et al. (2019)
G45076	TrGC	$ISOPDO2 \rightarrow MACR + HCHO + OH$	KHSD	Sander et al. (2019)
G45077a	TrGC	$ZC0DC23DBC0OH + OH \rightarrow .6 C10DC2O2C40OH + .4 C10OHC2O2C40D$	$k_adt*a_cho*a_ch2ooh$	Sander et al. (2019)
G45077b	TrGC	$ZC0DC23DBC0OH + OH \rightarrow .6 C10DC3O2C40OH + .4 C10OHC3O2C40D$	$k_ads*a_cho*a_ch2ooh$	Sander et al. (2019)
G45077c	TrGC	$ZC0DC23DBC0OH + OH \rightarrow LZCO3HC23DBC0D$	$k_t*f_o*f_alk+0.6*k_CH30OH_OH$	Sander et al. (2019)
G45077d	TrGC	$ZC0DC23DBC0OH + OH \rightarrow C4MDIAL + OH$	$k_s*f_sooh*f_allyl$	Sander et al. (2019)
G45078	TrGC	$ZC0DC23DBC0OH + O_3 \rightarrow .4672 OH + .2336 HCOCOCH_2O_2 + .2336 CO + .2336 CH_3C(O) + .4672 HOOCH_2CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH_2CHO + .02765 H_2O_2 + .02592 CH_3OOH + .02592 CO_2 + .01037 HCOCO + .01555 CH_2OO + .01555 CO + .006908 HOOCH_2CO_3 + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH_2OOH + .2628 GLYOX + .0972 CH_3COCH_2O_2H + .00972 HCOCO_2H + .005832 GLYOX + .005832 H_2O_2 + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO_2 + .01458 HCOOH + .01458 CO$	2.4E-17	Sander et al. (2019)
G45079	TrGC	$C10OHC2O2C40D \rightarrow .78 CH_3COCH_2O_2H + .78 HOCHCHO + .22 CO_2H_3CHO + .22 HCHO + .22 OH$	$k1_R02t0R02$	Sander et al. (2019)
G45080	TrGCN	$C10OHC2O2C40D + NO \rightarrow .78 CH_3COCH_2O_2H + .78 HOCHCHO + .22 CO_2H_3CHO + .22 HCHO + .22 OH + NO_2$	KR02N0	Sander et al. (2019)*
G45081a	TrGC	$C10OHC2O2C40D + HO_2 \rightarrow C10OHC2OOHC40D$	$KR02H02(5)*rcoch2o2_ooh$	Sander et al. (2019)
G45081b	TrGC	$C10OHC2O2C40D + HO_2 \rightarrow .78 CH_3COCH_2O_2H + .78 HOCHCHO + .22 CO_2H_3CHO + .22 HCHO + 1.22 OH$	$KR02H02(5)*rcoch2o2_oh$	Sander et al. (2019)
G45082	TrGC	$C10OHC2O2C40D \rightarrow CH_3COCH_2O_2H + GLYOX + OH$	KHSB	Sander et al. (2019)
G45083	TrGC	$C10DC2O2C40OH \rightarrow OH + C10DC2OOHC40D$	K15HSDHB	Sander et al. (2019)
G45084a	TrGC	$C10OHC2OOHC40D + OH \rightarrow C10DC2OOHC40D + OH$	$2.*k_s*f_sooh*f_tch2oh$	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45084b	TrGC	$C10OHC2OOHC4OD + OH \rightarrow CH_3COCH_2O_2H + 2 CO + 2 HO_2 + OH$	$k_t*f_toh*f_pch2oh*f_pch2oh$	Sander et al. (2019)
G45084c	TrGC	$C10OHC2OOHC4OD + OH \rightarrow C10OHC2O2C4OD$	$0.6*k_CH300H_OH$	Sander et al. (2019)
G45085	TrGC	$C1ODC2OOHC4OD + OH \rightarrow CO_2H_3CHO + CO + H_2O + OH$	$k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho$	Sander et al. (2019)
G45086	TrGC	$C1ODC3O2C4OOH \rightarrow MGLYOX + HOOCH_2CHO + HO_2$	$k1_R02s0R02$	Sander et al. (2019)
G45087	TrGCN	$C1ODC3O2C4OOH + NO \rightarrow MGLYOX + HOOCH_2CHO + HO_2 + NO_2$	KR02N0	Sander et al. (2019)
G45088	TrGC	$C1ODC3O2C4OOH + HO_2 \rightarrow .5 CH_3C(O) + .5 CO + .5 MGLYOX + .5 HO_2 + HOOCH_2CO_3$	KR02H02(5)	Sander et al. (2019)
G45089	TrGC	$C1ODC3O2C4OOH \rightarrow MGLYOX + OH + HOOCH_2CHO$	KHSD	Sander et al. (2019)
G45090	TrGC	$C10OHC3O2C4OD \rightarrow .625 MGLYOX + 2 CO + 1.625 HO_2 + .375 CH_3C(O) + .375 CO_2 + OH$	K15HSDHB	Sander et al. (2019)
G45091	TrGC	$LHC4ACCO_3 \rightarrow LZCO_3HC_2_3DBCOD + HO_2$	K16HS	Sander et al. (2019)
G45092a	TrGC	$C4MDIAL + OH \rightarrow C1ODC2O2C4OD$	$(k_adt+k_ads)*a_cho*a_cho$	Sander et al. (2019)*
G45092b	TrGC	$C4MDIAL + OH \rightarrow ZCO_3C_2_3DBCOD$	$2*k_t*f_o*f_alk$	Sander et al. (2019)*
G45093	TrGCN	$C4MDIAL + NO_3 \rightarrow ZCO_3C_2_3DBCOD + HNO_3$	$KN03AL*4.25*2.$	Sander et al. (2019)*
G45094a	TrGC	$C1ODC2O2C4OD + HO_2 \rightarrow OH + MGLYOX + HOCHCHO$	$KR02H02(5)*rcoch2o2_oh$	Sander et al. (2019)
G45094b	TrGC	$C1ODC2O2C4OD + HO_2 \rightarrow C1ODC2OOHC4OD$	$KR02H02(5)*rcoch2o2_ooh$	Sander et al. (2019)
G45095	TrGCN	$C1ODC2O2C4OD + NO \rightarrow NO_2 + MGLYOX + HOCHCHO$	KR02N0	Sander et al. (2019)*
G45096	TrGC	$C1ODC2O2C4OD \rightarrow MGLYOX + HOCHCHO$	$k1_R02t0R02$	Sander et al. (2019)
G45097a	TrGC	$C1ODC2OOHC4OD + OH \rightarrow MGLYOX + 2 CO$	$(2.*k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_cho*f_pch2oh)*.5$	Sander et al. (2019)
G45097b	TrGC	$C1ODC2OOHC4OD + OH \rightarrow MGLYOX + 2 CO + OH$	$(2.*k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_cho*f_pch2oh)*.5$	Sander et al. (2019)
G45098	TrGCN	$LISOPACNO_3O_2 + NO \rightarrow .21 NOA + .21 HOCH_2CHO + .21 HO_2 + .49 HO_1_2CO_3C_4 + .49 HCHO + .49 NO_2 + .045 MVKNO_3 + .045 HCHO + .255 CH_3COCH_2OH + .255 NO_3CH_2CHO + .225 H_2O_2 + NO_2$	KR02N0	Sander et al. (2019)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45099	TrGCN	LISOPACNO3O2 → .21 NOA + .21 HOCH ₂ CHO + .21 HO ₂ + .49 HO12CO3C4 + .49 HCHO + .49 NO ₂ + .045 MVKNO3 + .045 HCHO + .255 CH ₃ COCH ₂ OH + .255 NO ₃ CH ₂ CHO + .225 H ₂ O ₂	k1_R02t0R02+KR02H02(5)*c(ind_H02)	Sander et al. (2019)
G45100	TrGCN	ISOPBDNO3O2 + NO → .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO ₂ + 1.6 NO ₂	KR02N0	Sander et al. (2019)*
G45101	TrGCN	ISOPBDNO3O2 → .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO ₂ + .6 NO ₂	k1_R02s0R02+KR02H02(5)*c(ind_H02)	Sander et al. (2019)
G45102	TrGCN	LISOPACNO3 + O ₃ → .8704 OH + .365 HO ₂ + .73 MGLYOX + .4325 NO ₃ CH ₂ CHO + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .4325 NO ₂ + .0891 H ₂ O ₂ + .135 NOA + .0675 HOCHCHO + .3866 HOCH ₂ CHO + .0405 CH ₃ OH + .0405 CO + .0054 HOCH ₂ CO	2.8E-17	Feierabend et al. (2008), Sander et al. (2019)
G45103	TrGC	DB1O2 → DB1O2	k1_R02s0R02	Sander et al. (2019)
G45104a	TrGC	DB1O2 + HO ₂ → DB1OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2019)*
G45104b	TrGC	DB1O2 + HO ₂ → DB1O2 + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2019)
G45105a	TrGCN	DB1O2 + NO → DB1O2 + NO ₂	KR02N0*(1.-alpha_AN(7,2,0,0,0,temp,cair))	Sander et al. (2019)
G45105b	TrGCN	DB1O2 + NO → DB1NO3	KR02N0*alpha_AN(7,2,0,0,0,temp,cair)	Sander et al. (2019)
G45106	TrGCN	DB1O2 + NO ₃ → DB1O2 + NO ₂	KR02N03	Sander et al. (2019)
G45107	TrGC	DB1O2 → DB1O2 + OH	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 → DB1O2	KDEC*0.72	see note*
G45108b	TrGC	DB1O2 → .5 HVMK + .5 HMAC + HCHO + HO ₂	KDEC*0.28	see note*
G45109	TrGC	DB1O2 → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂	k1_R02s0R02	Sander et al. (2019)
G45110a	TrGC	DB1O2 + HO ₂ → DB2OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2019)
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	Sander et al. (2019)
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	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45113	TrGC	DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH	K14HSAL	Sander et al. (2019)
G45114a	TrGC	DB1OOH + OH → DB1O2	.6*k_CH300H_OH	Sander et al. (2019)
G45114b	TrGC	DB1OOH + OH → HCOOH + HO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2019)*
G45115	TrGC	DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH	4.67E-26*temp**3.286*EXP(4509./ (1.987*temp))	Sander et al. (2019), da Silva (2010)*
G45116	TrGCN	DB1NO3 + OH → HCOOH + NO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2019)*
G45117	TrGC	DB2OOH + OH → DB1O2	.6*k_CH300H_OH	Sander et al. (2019)*
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	Sander et al. (2019)
G45119a	TrGC	LZCO3HC23DBCOD + OH → .62 CO ₂ H ₃ CHO + .62 OH + .62 CO ₂ + .38 MGLYOX + .38 HCOCO ₃ H + .38 HO ₂	k_adt*a_cho*a_co2h	Sander et al. (2019)
G45119b	TrGC	LZCO3HC23DBCOD + OH → .62 CH ₃ COCO ₃ H + 1.24 CO + 1.24 HO ₂ + .38 MGLYOX + .38 HO ₂ + .38 CO + .38 HO ₂ + .38 OH + .38 CO ₂	k_ads*a_cho*a_co2h	Sander et al. (2019)
G45120	TrGC	LISOPEFO ₂ → LISOPEFO	k1_R02pOR02	Sander et al. (2019)
G45121a	TrGCN	LISOPEFO ₂ + NO → LISOPEFO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Sander et al. (2019)
G45121b	TrGCN	LISOPEFO ₂ + NO → ISOPDNO ₃	KR02N0*alpha_AN(6,1,0,0,0,temp, cair)	Sander et al. (2019)*
G45122a	TrGC	LISOPEFO ₂ + HO ₂ → .7143 ISOPDOOH + .2857 ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2019)
G45122b	TrGC	LISOPEFO ₂ + HO ₂ → LISOPEFO + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2019)
G45123	TrGCN	LISOPEFO ₂ + NO ₃ → LISOPEFO + NO ₂	KR02N03	Sander et al. (2019)
G45124	TrGC	LISOPEFO ₂ → .7143 MACR + .2857 MVK + HCHO + OH	.7143*KHSD+.2857*KHSB	Sander et al. (2019)
G45125	TrGC	LISOPEFO → .7143 MACR + .2857 MVK + HCHO + HO ₂	KDEC	Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45126a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	3METHYLFURAN + OH → L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Sander et al. (2019)*
G45129	TrGCN	3METHYLFURAN + NO ₃ → L3METHYLFURANO2 + NO ₂	1.9E-11	Sander et al. (2019), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 → C4MDIAL + HO ₂	k1_R02sOR02	Sander et al. (2019)
G45131	TrGCN	L3METHYLFURANO2 + NO → C4MDIAL + HO ₂ + NO ₂	KR02NO	Sander et al. (2019)*
G45132	TrGC	L3METHYLFURANO2 + HO ₂ → C4MDIAL + HO ₂	KR02H02(5)	Sander et al. (2019)*
G45133	TrGC	ZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂	k1_R02RC03	Sander et al. (2019)
G45134a	TrGC	ZCO3C23DBCOD + HO ₂ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH	KAPH02*rco3_oh	Sander et al. (2019)
G45134b	TrGC	ZCO3C23DBCOD + HO ₂ → LZCO3HC23DBCOD	KAPH02*(rco3_oh+rco3_o3)	Sander et al. (2019)*
G45135	TrGCN	ZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KAPNO	Sander et al. (2019)
G45136	TrGCN	ZCO3C23DBCOD + NO ₂ → ZCPANC23DBCOD	k_CH3C03_NO2	Rickard and Pascoe (2009)
G45137	TrGCN	ZCO3C23DBCOD + NO ₃ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	1.6*KR02N03	Sander et al. (2019)
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	Sander et al. (2019)*
G45200	TrGTerC	C511O2 → CH ₃ C(O) + HCOCH2CHO	k1_R02sOR02	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO → CH ₃ C(O) + HCOCH2CHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45202a	TrGTerC	$C511O2 + HO_2 \rightarrow C511OOH$	$KR02H02(5)*rcoch2o2_ooh$	Rickard and Pascoe (2009), Sander et al. (2019)
G45202b	TrGTerC	$C511O2 + HO_2 \rightarrow CH_3C(O) + HCOCH_2CHO + OH$	$KR02H02(5)*rcoch2o2_oh$	Rickard and Pascoe (2009), Sander et al. (2019)
G45203	TrGTerC	$C511OOH + OH \rightarrow C511O2$	7.49E-11	Rickard and Pascoe (2009)
G45204	TrGTerC	$CO23C4CHO + OH \rightarrow CO23C4CO3$	6.65E-11	Rickard and Pascoe (2009)
G45205	TrGTerCN	$CO23C4CHO + NO_3 \rightarrow CO23C4CO3 + HNO_3$	$KN03AL*5.5$	Rickard and Pascoe (2009)
G45206	TrGTerC	$CO23C4CO3 \rightarrow CH_3COCOCH_2O_2 + CO_2$	$k1_R02RC03$	Rickard and Pascoe (2009)
G45207	TrGTerCN	$CO23C4CO3 + NO \rightarrow CH_3COCOCH_2O_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)*
G45208	TrGTerCN	$CO23C4CO3 + NO_2 \rightarrow C5PAN9$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45209a	TrGTerC	$CO23C4CO3 + HO_2 \rightarrow CO23C4CO3H$	$KAPH02*(rco3_ooh+rco3_o3)$	Rickard and Pascoe (2009)
G45209b	TrGTerC	$CO23C4CO3 + HO_2 \rightarrow CH_3COCOCH_2O_2 + CO_2 + OH$	$KAPH02*rco3_oh$	Rickard and Pascoe (2009)
G45210	TrGTerCN	$C5PAN9 \rightarrow CO23C4CO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G45211	TrGTerCN	$C5PAN9 + OH \rightarrow CH_3COCOCHO + CO + NO_2$	3.12E-13	Rickard and Pascoe (2009)
G45212	TrGTerC	$C512O2 \rightarrow C513O2$	$k1_R02pR02$	Rickard and Pascoe (2009)
G45213	TrGTerC	$C512O2 + HO_2 \rightarrow C512OOH$	$KR02H02(5)$	Rickard and Pascoe (2009)
G45214	TrGTerCN	$C512O2 + NO \rightarrow C513O2 + NO_2$	$KR02N0$	Rickard and Pascoe (2009)*
G45215	TrGTerC	$C512OOH + OH \rightarrow CO13C4CHO + OH$	1.01E-10	Rickard and Pascoe (2009)
G45216	TrGTerC	$C513O2 \rightarrow GLYOX + HOC_2H_4CO_3$	$k1_R02sOR02$	Rickard and Pascoe (2009)
G45217	TrGTerCN	$C513O2 + NO \rightarrow GLYOX + HOC_2H_4CO_3 + NO_2$	$KR02N0$	Rickard and Pascoe (2009)*
G45218a	TrGTerC	$C513O2 + HO_2 \rightarrow C513OOH$	$KR02H02(5)*rcoch2o2_ooh$	Rickard and Pascoe (2009), Sander et al. (2019)
G45218b	TrGTerC	$C513O2 + HO_2 \rightarrow GLYOX + HOC_2H_4CO_3 + OH$	$KR02H02(5)*rcoch2o2_oh$	Rickard and Pascoe (2009), Sander et al. (2019)
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	$CHOC3COCO3 \rightarrow CHOC3COO2 + CO_2$	$k1_R02RC03$	Rickard and Pascoe (2009)
G45223	TrGTerC	$CHOC3COCO3 + HO_2 \rightarrow CHOC3COOOH$	KAPH02	Rickard and Pascoe (2009)
G45224	TrGTerCN	$CHOC3COCO3 + NO_2 \rightarrow CHOC3COPAN$	k_CH3C03_N02	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	$C514O2 + NO \rightarrow CO13C4CHO + HO_2 + NO_2$	$KR02N0*(1.-alpha_AN(7,2,0,1,0, temp, cair))$	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45228b	TrGTerCN	$C514O2 + NO \rightarrow C514NO3$	$KR02N0*\alpha_{AN}(7,2,0,1,0,temp,cair)$	Rickard and Pascoe (2009), Sander et al. (2019)
G45229	TrGTerCN	$C514O2 + NO_3 \rightarrow CO13C4CHO + HO_2 + NO_2$	KR02N03	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), Sander et al. (2019)*
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), Sander et al. (2019)
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), Sander et al. (2019)
G45238	TrGTerCN	$MBO + NO_3 \rightarrow LNMBOABO2$	$4.6E-14*EXP(-400./TEMP)$	Rickard and Pascoe (2009), Sander et al. (2019)
G45239	TrGTerC	$LMBOABO2 + HO_2 \rightarrow LMBOABOOH$	KR02H02(5)	Rickard and Pascoe (2009), Sander et al. (2019)
G45240a	TrGTerCN	$LMBOABO2 + NO \rightarrow LMBOABNO3$	$KR02N0*(.67*\alpha_{AN}(7,2,0,0,0,temp,cair)+.33*\alpha_{AN}(7,1,0,0,0,temp,cair))$	Rickard and Pascoe (2009), Sander et al. (2019)
G45240b	TrGTerCN	$LMBOABO2 + NO \rightarrow HOCH_2CHO + CH_3COCH_3 + HO_2 + NO_2$	$KR02N0*(1-(.67*\alpha_{AN}(7,2,0,0,0,temp,cair)+.33*\alpha_{AN}(7,1,0,0,0,temp,cair)))*.67$	Rickard and Pascoe (2009), Sander et al. (2019)
G45240c	TrGTerCN	$LMBOABO2 + NO \rightarrow IBUTALOH + HCHO + HO_2 + NO_2$	$KR02N0*(1-(.67*\alpha_{AN}(7,2,0,0,0,temp,cair)+.33*\alpha_{AN}(7,1,0,0,0,temp,cair)))*.33$	Rickard and Pascoe (2009), Sander et al. (2019)
G45241a	TrGTerC	$LMBOABO2 \rightarrow HOCH_2CHO + CH_3COCH_3 + HO_2$	$k1_R02sOR02*.67$	Rickard and Pascoe (2009), Sander et al. (2019)
G45241b	TrGTerC	$LMBOABO2 \rightarrow IBUTALOH + HCHO + HO_2$	$k1_R02pOR02*.33$	Rickard and Pascoe (2009), Sander et al. (2019)
G45242a	TrGTerC	$LMBOABOOH + OH \rightarrow MBOACO$	$.67*2.93E-11+.33*2.05E-12$	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45242b	TrGTerC	LMBOABOOH + OH → LMBOABO2	.6*k_CH300H_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45243	TrGTerCN	LMBOABNO3 + OH → MBOACO + NO ₂	.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45244	TrGTerC	MBOACO + OH → MBOCOCO + HO ₂	3.79E-12	Rickard and Pascoe (2009)
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), Sander et al. (2019)
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), Sander et al. (2019)*
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), Sander et al. (2019)
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_R02sOR02	Rickard and Pascoe (2009), Sander et al. (2019)
G45250a	TrGTerCN	LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBCO	.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45250b	TrGTerCN	LNMBOABOOH + OH → LNMBOABO2	.6*k_CH300H_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45251	TrGTerCN	NMBOBCO + OH → NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45252a	TrGTerCN	NC4OHCO3 + HO ₂ → IBUTALOH + CO ₂ + NO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G45252b	TrGTerCN	NC4OHCO3 + HO ₂ → NC4OHCO3H	KAPH02*(rco3_o3+rco3_ooH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45253	TrGTerCN	NC4OHCO3 + NO → IBUTALOH + CO ₂ + NO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G45254	TrGTerCN	NC4OHCO3 + NO ₂ → NC4OHCPAN	k_CH3C03_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_R02RC03	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), Sander et al. (2019)
G45400	TrGAroCN	NC4MDCO2HN + OH → MMALANHY + NO ₂	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45401	TrGAroCN	$C54CO + NO_3 \rightarrow 3 CO + CH_3C(O)OO + HNO_3$	$KNO3AL*5.5$	Rickard and Pascoe (2009)
G45402	TrGAroC	$C54CO + OH \rightarrow 3 CO + CH_3C(O)OO$	$1.72E-11$	Rickard and Pascoe (2009)
G45403a	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow NTLFUOOH$	$KR02H02(5)*(1-rcoch2o2_oh)$	Rickard and Pascoe (2009)
G45403b	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow ACCOMECHO + NO_2 + OH$	$KR02H02(5)*rcoch2o2_oh$	Rickard and Pascoe (2009)
G45404	TrGAroCN	$NTLFUO2 + NO \rightarrow ACCOMECHO + NO_2 + NO_2$	$KR02N0$	Rickard and Pascoe (2009)*
G45405	TrGAroCN	$NTLFUO2 + NO_3 \rightarrow ACCOMECHO + NO_2 + NO_2$	$KR02N03$	Rickard and Pascoe (2009)*
G45406	TrGAroCN	$NTLFUO2 \rightarrow ACCOMECHO + NO_2$	$k1_R02t0R02$	Rickard and Pascoe (2009)*
G45407	TrGAroC	$C5134CO2OH + OH \rightarrow C54CO + HO_2$	$7.48E-11$	Rickard and Pascoe (2009)
G45408	TrGAroCN	$C5COO2NO2 + OH \rightarrow MGLYOX + CO + CO + NO_2$	$5.43E-11$	Rickard and Pascoe (2009)
G45409	TrGAroCN	$C5COO2NO2 \rightarrow C5CO14O2 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45410	TrGAroC	$C5DIALOOH + OH \rightarrow C5DIALCO + OH$	$7.52E-11$	Rickard and Pascoe (2009)
G45411a	TrGAroC	$C4CO2DBC03 + HO_2 \rightarrow C4CO2DCO3H$	$KAPH02*(rco3_ooh+rco3_o3)$	Rickard and Pascoe (2009)
G45411b	TrGAroC	$C4CO2DBC03 + HO_2 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + OH$	$KAPH02*rco3_oh$	Rickard and Pascoe (2009), Sander et al. (2019)
G45412	TrGAroCN	$C4CO2DBC03 + NO \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	$KAPN0$	Rickard and Pascoe (2009)
G45413	TrGAroCN	$C4CO2DBC03 + NO_2 \rightarrow C4CO2DBPAN$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$C4CO2DBC03 + NO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	$KR02N03*1.74$	Rickard and Pascoe (2009)
G45415	TrGAroC	$C4CO2DBC03 \rightarrow HO_2 + CO + HCOCOCHO + CO_2$	$k1_R02RC03$	Rickard and Pascoe (2009)
G45416	TrGAroC	$MMALANHY + OH \rightarrow MMALANHYO2$	$1.50E-12$	Rickard and Pascoe (2009)
G45421a	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow MMALNHYOOH$	$KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh)$	Rickard and Pascoe (2009), Sander et al. (2019)
G45421b	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow CO2H3CO3 + CO_2 + OH$	$KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)$	Rickard and Pascoe (2009), Sander et al. (2019)
G45422	TrGAroCN	$MMALANHYO2 + NO \rightarrow CO2H3CO3 + CO_2 + NO_2$	$KR02N0$	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$MMALANHYO2 + NO_3 \rightarrow CO2H3CO3 + CO_2 + NO_2$	$KR02N03$	Rickard and Pascoe (2009)*
G45424	TrGAroC	$MMALANHYO2 \rightarrow CO2H3CO3 + CO_2$	$k1_R02t0R02$	Rickard and Pascoe (2009)*
G45428	TrGAroCN	$C4CO2DBPAN + OH \rightarrow HCOCOCHO + CO_2 + CO + NO_2$	$2.74E-11$	Rickard and Pascoe (2009)
G45429	TrGAroCN	$C4CO2DBPAN \rightarrow C4CO2DBC03 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	$C5CO14O2 + HO_2 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH$	$KAPH02*rco3_oh$	Rickard and Pascoe (2009)*
G45430b	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OH + O_3$	$KAPH02*rco3_o3$	Rickard and Pascoe (2009)
G45430c	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OOH$	$KAPH02*rco3_ooh$	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G45431	TrGAroCN	$C5CO14O2 + NO \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*
G45432	TrGAroCN	$C5CO14O2 + \text{NO}_2 \rightarrow C5COO2NO2$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45433	TrGAroCN	$C5CO14O2 + \text{NO}_3 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	$C5CO14O2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G45436	TrGAroC	$C5CO14OH + OH \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	$C5DICARB + \text{NO}_3 \rightarrow C5CO14O2 + \text{HNO}_3$	KN03AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	$C5DICARB + \text{O}_3 \rightarrow .5338 \text{ GLYOX} + .063 \text{ CH}_3\text{CHO} + .348 \text{ CH}_3\text{C(O)OO} + .918 \text{ CO} + .57 \text{ OH} + .473 \text{ HO}_2 + .0563 \text{ CH}_3\text{COCO}_2\text{H} + .5338 \text{ MGLYOX} + .676 \text{ H}_2\text{O}_2 + .063 \text{ HCHO} + .0563 \text{ HCOCO}_2\text{H} + .2465 \text{ CO}_2$	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	$C5DICARB + OH \rightarrow .48 \text{ C5CO14O2} + .52 \text{ C5DICARBO2}$	6.2E-11	Rickard and Pascoe (2009)
G45444	TrGAroC	$\text{MC3ODBCO}_2\text{H} + OH \rightarrow .35 \text{ GLYOX} + .35 \text{ CH}_3 + .35 \text{ CO} + .35 \text{ CO}_2 + .65 \text{ MMALANHY} + .65 \text{ HO}_2$	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	$\text{TLFUONE} + \text{NO}_3 \rightarrow \text{NTLFUO}_2$	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	$\text{TLFUONE} + \text{O}_3 \rightarrow .5 \text{ CO} + .5 \text{ OH} + .5 \text{ MECOACETO}_2 + .3125 \text{ C24O3CCO}_2\text{H} + .1875 \text{ ACCOMECHO} + .1875 \text{ H}_2\text{O}_2$	8.00E-19	see note*
G45453	TrGAroC	$\text{TLFUONE} + OH \rightarrow \text{TLFUO}_2$	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	$\text{ACCOMECO}_3 + \text{HO}_2 \rightarrow \text{ACCOMECO}_3\text{H}$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	$\text{ACCOMECO}_3 + \text{HO}_2 \rightarrow \text{MECOACETO}_2 + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45455	TrGAroCN	$\text{ACCOMECO}_3 + \text{NO} \rightarrow \text{MECOACETO}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	$\text{ACCOMECO}_3 + \text{NO}_2 \rightarrow \text{ACCOMEPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45457	TrGAroCN	$\text{ACCOMECO}_3 + \text{NO}_3 \rightarrow \text{MECOACETO}_2 + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	$\text{ACCOMECO}_3 \rightarrow \text{MECOACETO}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45459	TrGAroC	$\text{C4CO2DCO}_3\text{H} + OH \rightarrow \text{C4CO2DBC}_3$	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	$\text{ACCOMEOCHO} + \text{NO}_3 \rightarrow \text{ACCOMECO}_3 + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	$\text{ACCOMEOCHO} + OH \rightarrow \text{ACCOMECO}_3$	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	$\text{MMALNHYOOH} + OH \rightarrow \text{MMALANHYO}_2$	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	$\text{C5DICAROOH} + OH \rightarrow \text{C5134CO}_2\text{OH} + \text{OH}$	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	$\text{C5DICAROOH} + OH \rightarrow \text{C5DICARBO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G45468	TrGAroC	$\text{C24O3CCO}_2\text{H} + OH \rightarrow \text{MECOACETO}_2 + \text{CO}_2$	8.76E-13	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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 → ACCOMECO3 + 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	KR02N0	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 → ACCOMECO3	3.59E-12	Rickard and Pascoe (2009)
G45486a	TrGAroC	C5DIALO2 + HO ₂ → C5DIALOOH	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45486b	TrGAroC	C5DIALO2 + HO ₂ → MALDIAL + CO + HO ₂ + OH	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G45487	TrGAroCN	C5DIALO2 + NO → MALDIAL + CO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45488	TrGAroCN	C5DIALO2 + NO ₃ → MALDIAL + CO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G45489	TrGAroC	C5DIALO2 → MALDIAL + CO + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G45490a	TrGAroC	C5DICARBO2 + HO ₂ → C5DICAROOH	KR02H02(5)*(rco3_ooH+rco3_o3)	Rickard and Pascoe (2009)
G45491b	TrGAroC	C5DICARBO2 + HO ₂ → MGLYOX + GLYOX + HO ₂ + OH	KR02H02(5)*rco3_oh	Rickard and Pascoe (2009)*
G45492	TrGAroCN	C5DICARBO2 + NO → MGLYOX + GLYOX + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45493	TrGAroCN	C5DICARBO2 + NO ₃ → MGLYOX + GLYOX + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G45494	TrGAroC	C5DICARBO2 → MGLYOX + GLYOX + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G46200a	TrGTerC	CO235C6O2 + HO ₂ → CO235C6OOH	KR02H02(6)*rcoch2o2_ooH	Rickard and Pascoe (2009), Sander et al. (2019)
G46200b	TrGTerC	CO235C6O2 + HO ₂ → CO23C4CO3 + HCHO + OH	KR02H02(6)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G46201	TrGTerCN	CO235C6O2 + NO → CO23C4CO3 + HCHO + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46202	TrGTerC	CO235C6O2 → CO23C4CO3 + HCHO	k1_R02p0R02	Rickard and Pascoe (2009)
G46203	TrGTerC	CO235C6OOH + OH → CO235C6O2	1.01E-11	Rickard and Pascoe (2009)
G46204	TrGTerC	C614O2 → CO23C4CHO + HCHO + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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	$C614O2 + HO_2 \rightarrow C614OOH$	$KR02H02(6)*(1.-r_{chohch2o2_oh})$	Rickard and Pascoe (2009), Sander et al. (2019)
G46206b	TrGTerC	$C614O2 + HO_2 \rightarrow CO23C4CHO + HCHO + HO_2 + OH$	$KR02H02(6)*r_{chohch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2019)
G46207	TrGTerCN	$C614NO3 + OH \rightarrow C614CO + NO_2$	7.11E-12	Rickard and Pascoe (2009)
G46208	TrGTerC	$C614OOH + OH \rightarrow C614CO + OH$	8.69E-11	Rickard and Pascoe (2009)
G46209	TrGTerC	$C614CO + OH \rightarrow CO235C5CHO + HO_2$	3.22E-12	Rickard and Pascoe (2009)
G46210	TrGTerC	$CO235C5CHO + OH \rightarrow CO23C4CO3 + CO$	1.33E-11	Rickard and Pascoe (2009)
G46211	TrGTerCN	$CO235C5CHO + NO_3 \rightarrow CO23C4CO3 + CO + HNO_3$	$KN03AL*5.5$	Rickard and Pascoe (2009)
G46400	TrGAroC	$PHENOOH + OH \rightarrow PHENO2$	1.16E-10	Rickard and Pascoe (2009)
G46401	TrGAroC	$C6CO4DB + OH \rightarrow CO + CO + HO_2 + CO + HCOCOCHO$	7.70E-11	Rickard and Pascoe (2009)
G46402	TrGAroC	$C5CO2DCO3H + OH \rightarrow C5CO2DBC03$	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	$NDNPHENO2 + HO_2 \rightarrow NDNPHENOOH$	$KR02H02(6)*(1.-r_{chohch2o2_oh})$	Rickard and Pascoe (2009)
G46413b	TrGAroCN	$NDNPHENO2 + HO_2 \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH$	$KR02H02(6)*r_{chohch2o2_oh}$	Rickard and Pascoe (2009)*
G46414	TrGAroCN	$NDNPHENO2 + NO \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2$	$KR02N0$	Rickard and Pascoe (2009)*
G46415	TrGAroCN	$NDNPHENO2 + NO_3 \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2$	$KR02N03$	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46416	TrGAroCN	NDNPHEO2 → NC4DCO2H + HNO ₃ + CO + CO + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46417	TrGAroC	PBZQCO + OH → C5CO2OHCO3	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	CATECHOL + NO ₃ → CATEC1O + HNO ₃	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	CATECHOL + O ₃ → MALDALCO2H + HCOCO ₂ H + HO ₂ + OH	9.2E-18	Rickard and Pascoe (2009)
G46420	TrGAroC	CATECHOL + OH → CATEC1O	1.0E-10	Rickard and Pascoe (2009)
G46421	TrGAroC	C5COOHCO3H + OH → C5CO2OHCO3	8.01E-11	Rickard and Pascoe (2009)
G46422	TrGAroCN	NCATECHOL + NO ₃ → NNCATECO2	2.60E-12	Rickard and Pascoe (2009)
G46423	TrGAroCN	NCATECHOL + OH → NCATECO2	3.47E-12	Rickard and Pascoe (2009)
G46424a	TrGAroC	C5CO2OHCO3 + HO ₂ → C5COOHCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46424b	TrGAroC	C5CO2OHCO3 + HO ₂ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46425	TrGAroCN	C5CO2OHCO3 + NO → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46426	TrGAroCN	C5CO2OHCO3 + NO ₂ → C5CO2OH PAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46427	TrGAroCN	C5CO2OHCO3 + NO ₃ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46428	TrGAroC	C5CO2OHCO3 → HOCOC4DIAL + HO ₂ + CO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46429	TrGAroCN	BZEPOXMUC + NO ₃ → BZEMUCCO3 + HNO ₃	2*KNO3AL*2.75	Rickard and Pascoe (2009)
G46430	TrGAroC	BZEPOXMUC + O ₃ → EPXC4DIAL + .125 HCHO + .1125 HCOCO ₂ H + .0675 GLYOX + .0675 H ₂ O ₂ + .82 HO ₂ + .57 OH + 1.265 CO + .25 CO ₂	2.00E-18	Rickard and Pascoe (2009)*
G46431	TrGAroC	BZEPOXMUC + OH → .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard and Pascoe (2009)
G46432a	TrGAroCN	NCATECO2 + HO ₂ → NCATECOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	NCATECO2 + HO ₂ → NC4DCO2H + HCOCO ₂ H + HO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46433	TrGAroCN	NCATECO2 + NO → NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46434	TrGAroCN	NCATECO2 + NO ₃ → NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46435	TrGAroCN	NCATECO2 → NC4DCO2H + HCOCO ₂ H + HO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46436	TrGAroCN	NPHEN1OOH + OH → NPHEN1O2	9.00E-13	Rickard and Pascoe (2009)
G46437a	TrGAroCN	NPHENO2 + HO ₂ → NPHENOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46437b	TrGAroCN	NPHEN02 + HO ₂ → MALDALCO2H + GLYOX + NO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46438	TrGAroCN	NPHEN02 + NO → MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46439	TrGAroCN	NPHEN02 + NO ₃ → MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46440	TrGAroCN	NPHEN02 → MALDALCO2H + GLYOX + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46441	TrGAroC	BENZENE + OH → .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO ₂ + .53 PHENOL + .53 HO ₂	2.3E-12*EXP(-190/TEMP)	Rickard and Pascoe (2009)*
G46442	TrGAroCN	C5CO2OHPAN + OH → HOCOC4DIAL + CO + CO + NO ₂	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	C5CO2OHPAN → C5CO2OHCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G46444	TrGAroCN	CATEC1O + NO ₂ → NCATECHOL	k_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 NPHEO2	3.8E-12	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46458	TrGAroC	PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 HO ₂ + .14 PHENO2	4.7E-13*EXP(1220/TEMP)	Rickard and Pascoe (2009)*
G46459	TrGAroCN	PBZQONE + NO ₃ → NBZQO2	3.00E-13	Rickard and Pascoe (2009)
G46460	TrGAroC	PBZQONE + OH → PBZQO2	4.6E-12	Rickard and Pascoe (2009)
G46461a	TrGAroC	PHENO2 + HO ₂ → PHENOOH	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)*
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	C5CO2DBC03 + HO ₂ → C5CO2DCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBC03 + HO ₂ → CH ₃ C(O) + HCOCOCHO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBC03 + NO → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBC03 + NO ₂ → C5CO2DBPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBC03 + NO ₃ → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBC03 → CH ₃ C(O) + HCOCOCHO + CO ₂	k1_R02RC03	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_C6H502_N02	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_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O ₃ → C6H5O2	k_C6H50_03	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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46480a	TrGAroC	$\text{PBZQO}_2 + \text{HO}_2 \rightarrow \text{PBZQOOH}$	$\text{KR02H02}(6) * (1 - \text{rchohch2o2_oh} - \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)
G46480b	TrGAroC	$\text{PBZQO}_2 + \text{HO}_2 \rightarrow \text{C5CO2OHCO}_3 + \text{OH}$	$\text{KR02H02}(6) * (\text{rchohch2o2_oh} + \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)*
G46481	TrGAroCN	$\text{PBZQO}_2 + \text{NO} \rightarrow \text{C5CO2OHCO}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46482	TrGAroCN	$\text{PBZQO}_2 + \text{NO}_3 \rightarrow \text{C5CO2OHCO}_3 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46483	TrGAroC	$\text{PBZQO}_2 \rightarrow \text{C5CO2OHCO}_3$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46484	TrGAroC	$\text{BZOBIPEROH} + \text{OH} \rightarrow \text{MALDIALCO}_3 + \text{GLYOX}$	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	$\text{DNPHENO}_2 + \text{HO}_2 \rightarrow \text{DNPHENO}_2\text{OH}$	$\text{KR02H02}(6) * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G46485b	TrGAroCN	$\text{DNPHENO}_2 + \text{HO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{KR02H02}(6) * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G46486	TrGAroCN	$\text{DNPHENO}_2 + \text{NO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46487	TrGAroCN	$\text{DNPHENO}_2 + \text{NO}_3 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46488	TrGAroCN	$\text{DNPHENO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	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	$\text{BZEMUCO}_2 + \text{HO}_2 \rightarrow \text{BZEMUCOOH}$	KR02H02(6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	$\text{BZEMUCO}_2 + \text{HO}_2 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{OH}$	KR02H02(6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO} \rightarrow \text{BZEMUCNO}_3$	$\text{KR02N0} * \alpha_{\text{AN}}(10, 2, 0, 1, 0, \text{temp, cair})$	Rickard and Pascoe (2009)
G46491b	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO} \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(10, 2, 0, 1, 0, \text{temp, cair}))$	Rickard and Pascoe (2009)*
G46492	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO}_3 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46493	TrGAroC	$\text{BZEMUCO}_2 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO}$	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	$\text{C5CO2DBPAN} \rightarrow \text{C5CO2DBC}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	$\text{NBZQOOH} + \text{OH} \rightarrow \text{NBZQO}_2$	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	$\text{CATEC1OOH} + \text{OH} \rightarrow \text{CATEC1O}_2$.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46498	TrGAroC	$\text{C6125CO} + \text{OH} \rightarrow \text{C5CO14O}_2 + \text{CO}$	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	$\text{NBZQO}_2 + \text{HO}_2 \rightarrow \text{NBZQOOH}$	$\text{KR02H02}(6) * (1 - \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46499b	TrGAroCN	NBZQO2 + HO ₂ → C6CO4DB + NO ₂ + OH	KR02H02(6)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G46500	TrGAroCN	NBZQO2 + NO → C6CO4DB + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46501	TrGAroCN	NBZQO2 + NO ₃ → C6CO4DB + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46502	TrGAroCN	NBZQO2 → C6CO4DB + NO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G46503	TrGAroCN	DNPHENO0H + OH → DNPHENO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46504	TrGAroC	CATEC1O2 + HO ₂ → CATEC1OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46505a	TrGAroCN	CATEC1O2 + NO → CATEC1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46505b	TrGAroCN	CATEC1O2 + NO ₂ → CATEC1O + NO ₃	K_C6H502_N02	Jagiella and Zabel (2007)*
G46506	TrGAroCN	CATEC1O2 + NO ₃ → CATEC1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46507	TrGAroC	CATEC1O2 → CATEC1O	k1_R02s0R02	Rickard and Pascoe (2009)
G46508	TrGAroC	BZEMUCCO3H + OH → BZEMUCCO3	4.37E-11	Rickard and Pascoe (2009)
G46509	TrGAroC	C6H5OOH + OH → C6H5O2	3.60E-12	Rickard and Pascoe (2009)
G46510	TrGAroC	BZEMUCOOH + OH → BZEMUCCO + OH	1.31E-10	Rickard and Pascoe (2009)
G46511a	TrGAroC	BZEMUCCO3 + HO ₂ → BZEMUCCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G46511b	TrGAroC	BZEMUCCO3 + HO ₂ → BZEMUCCO3H	KAPH02*rco3_ooH	Rickard and Pascoe (2009)
G46511c	TrGAroC	BZEMUCCO3 + HO ₂ → C5DIALO2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46512	TrGAroCN	BZEMUCCO3 + NO → C5DIALO2 + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46513	TrGAroCN	BZEMUCCO3 + NO ₂ → BZEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G46514	TrGAroCN	BZEMUCCO3 + NO ₃ → C5DIALO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46515	TrGAroC	BZEMUCCO3 → C5DIALO2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G46516	TrGAroC	C6H5O2 + HO ₂ → C6H5OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46517a	TrGAroCN	C6H5O2 + NO → C6H5O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46517b	TrGAroCN	C6H5O2 + NO ₂ → C6H5O + NO ₃	K_C6H502_N02	Jagiella and Zabel (2007)*
G46518	TrGAroCN	C6H5O2 + NO ₃ → C6H5O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46519	TrGAroC	C6H5O2 → C6H5O	k1_R02sR02	Rickard and Pascoe (2009)
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO ₂	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	BZBIPERO2 + HO ₂ → BZBIPEROOH	KR02H02(6)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G46522b	TrGAroC	BZBIPERO2 + HO ₂ → OH + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02H02(6)*rbipero2_oh	Rickard and Pascoe (2009), Bird- sall et al. (2010)*
G46523a	TrGAroCN	BZBIPERO2 + NO → BZBIPERNO3	KR02N0*alpha_AN(9,2,0,0,1,temp, cair)	Rickard and Pascoe (2009)
G46523b	TrGAroCN	BZBIPERO2 + NO → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N0*(1.-alpha_AN(9,2,0,0,1, temp,cair))	Rickard and Pascoe (2009)*
G46524	TrGAroCN	BZBIPERO2 + NO ₃ → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N03	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G46525	TrGAroC	BZBIPERO2 → GLYOX + HO ₂ + BZFUONE	k1_R02s0R02	Rickard and Pascoe (2009)*
G47200	TrGTerCN	CO235C6CHO + NO ₃ → CO235C6CO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	CO235C6CO3 + HO ₂ → C235C6CO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO ₂ → CO235C6O2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47203	TrGTerCN	CO235C6CO3 + NO → CO235C6O2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G47204	TrGTerCN	CO235C6CO3 + NO ₂ → C7PAN3	k_CH3C03_NO2	Rickard and Pascoe (2009)
G47205	TrGTerC	CO235C6CO3 → CO235C6O2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G47206	TrGTerC	C235C6CO3H + OH → CO235C6CO3	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	C7PAN3 + OH → CO235C5CHO + CO + NO ₂	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	C7PAN3 → CO235C6CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G47209a	TrGTerC	C716O2 + HO ₂ → C716OOH	KR02H02(7)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2019)
G47209b	TrGTerC	C716O2 + HO ₂ → CO13C4CHO + CH ₃ C(O) + OH	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G47210	TrGTerCN	C716O2 + NO → CO13C4CHO + CH ₃ C(O) + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47211	TrGTerC	C716O2 → CO13C4CHO + CH ₃ C(O)	k1_R02s0R02	Rickard and Pascoe (2009)
G47212	TrGTerC	C716OOH + OH → CO235C6CHO + OH	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	C721O2 + HO ₂ → C721OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	C721O2 + NO → C722O2 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47215	TrGTerC	C721O2 → C722O2	k1_R02pR02	Rickard and Pascoe (2009)
G47216	TrGTerC	C721OOH + OH → C721O2	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	C722O2 + HO ₂ → C722OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	C722O2 + NO → CH ₃ COCH ₃ + C44O2 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47219	TrGTerC	C722O2 → CH ₃ COCH ₃ + C44O2	k1_R02tR02	Rickard and Pascoe (2009)
G47220	TrGTerC	C722OOH + OH → C722O2	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	ROO6R3O2 → ROO6R5O2	5.68E10*EXP(-8745./TEMP)	Vereecken and Peeters (2012)
G47222	TrGTerCN	ROO6R3O2 + NO → ROO6R3O + NO ₂	KR02NO	Vereecken and Peeters (2012)*
G47223	TrGTerC	ROO6R3O2 + HO ₂ → 7 LCARBON	KR02H02(7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	ROO6R3O2 → ROO6R3O	k1_R02sR02	Vereecken and Peeters (2012)
G47225	TrGTerC	ROO6R3O → 7 LCARBON + HO ₂	5.7E10*EXP(-2949./TEMP)	Vereecken and Peeters (2012)*
G47226	TrGTerC	ROO6R5O2 → 7 LCARBON + OH	9.17E10*EXP(-8706./TEMP)	Vereecken and Peeters (2012)*
G47400	TrGAroC	TOLUENE + OH → .07 C6H5CH2O2 + .18 CRESOL + .18 HO ₂ + .65 TLBIPERO2 + .10 TLEPOXMUC + .10 HO ₂	1.8E-12*EXP(340/TEMP)	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G47401	TrGAroC	$C_6H_5CH_2O_2 + HO_2 \rightarrow C_6H_5CH_2OOH$	$1.5E-13 * EXP(1310/TEMP)$	Rickard and Pascoe (2009)
G47402a	TrGAroCN	$C_6H_5CH_2O_2 + NO \rightarrow C_6H_5CH_2NO_3$	$KR02N0 * \alpha_AN(7, 1, 0, 0, 0, temp, cair)$	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	$C_6H_5CH_2O_2 + NO \rightarrow BENZAL + HO_2 + NO_2$	$KR02N0 * (1. - \alpha_AN(7, 1, 0, 0, 0, temp, cair))$	Rickard and Pascoe (2009)*
G47403	TrGAroCN	$C_6H_5CH_2O_2 + NO_3 \rightarrow BENZAL + HO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)*
G47404	TrGAroC	$C_6H_5CH_2O_2 \rightarrow BENZAL + HO_2$	$2. * (k_CH302 * 2.4E-14 * EXP(1620./TEMP)) * 0.5 * R02$	Rickard and Pascoe (2009)*
G47405	TrGAroCN	$CRESOL + NO_3 \rightarrow .103 CRESO_2 + .103 HNO_3 + .506 NCRESO_2 + .391 TOLIO + .391 HNO_3$	$1.4E-11$	Rickard and Pascoe (2009)*
G47406	TrGAroC	$CRESOL + OH \rightarrow .2 CRESO_2 + .727 MCATECHOL + .727 HO_2 + .073 TOLIO$	$4.65E-11$	Rickard and Pascoe (2009)*
G47407a	TrGAroC	$TLBIPERO_2 + HO_2 \rightarrow TLBIPEROOH$	$KR02H02(7) * (1. - rbipero2_oh)$	Rickard and Pascoe (2009)
G47407b	TrGAroC	$TLBIPERO_2 + HO_2 \rightarrow OH + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL$	$KR02H02(7) * rbipero2_oh$	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G47408a	TrGAroCN	$TLBIPERO_2 + NO \rightarrow NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL$	$KR02N0 * (1. - \alpha_AN(11, 2, 0, 0, 1, temp, cair))$	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	$TLBIPERO_2 + NO \rightarrow TLBIPERNO_3$	$KR02N0 * \alpha_AN(11, 2, 0, 0, 1, temp, cair)$	Rickard and Pascoe (2009)*
G47409	TrGAroCN	$TLBIPERO_2 + NO_3 \rightarrow NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL$	KR02N03	Rickard and Pascoe (2009)*
G47410	TrGAroC	$TLBIPERO_2 \rightarrow .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL$	$k1_R02sOR02$	Rickard and Pascoe (2009)*
G47411	TrGAroCN	$TLEPOXMUC + NO_3 \rightarrow TLEMUCCO_3 + HNO_3$	$KN03AL * 2.75$	Rickard and Pascoe (2009)
G47412	TrGAroC	$TLEPOXMUC + O_3 \rightarrow EPXC4DIAL + .125 CH_3CHO + .695 CH_3C(O) + .57 CO + .57 OH + .125 HO_2 + .1125 CH_3COCO_2H + .0675 MGLYOX + .0675 H_2O_2 + .25 CO_2$	$5.00E-18$	Rickard and Pascoe (2009)*
G47413	TrGAroC	$TLEPOXMUC + OH \rightarrow .31 TLEMUCCO_3 + .69 TLEMUCO_2$	$7.99E-11$	Rickard and Pascoe (2009)*
G47414	TrGAroC	$C_6H_5CH_2OOH + OH \rightarrow BENZAL + OH$	$2.05E-11$	Rickard and Pascoe (2009)
G47415	TrGAroCN	$C_6H_5CH_2NO_3 + OH \rightarrow BENZAL + NO_2$	$6.03E-12$	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G47416	TrGAroCN	BENZAL + NO ₃ → C ₆ H ₅ CO ₃ + HNO ₃	2.40E-15	Rickard and Pascoe (2009)
G47417	TrGAroC	BENZAL + OH → C ₆ H ₅ CO ₃	5.9E-12*EXP(225/TEMP)	Rickard and Pascoe (2009)
G47418a	TrGAroC	CRESO ₂ + HO ₂ → CRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO ₂ + HO ₂ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO ₂ + NO → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO ₂ + NO ₃ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47421	TrGAroC	CRESO ₂ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO ₂ + HO ₂ → NCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO ₂ + HO ₂ → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO ₂ + NO → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO ₂ + NO ₃ → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO ₂ → C ₅ CO ₁₄ OH + GLYOX + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47426	TrGAroCN	TOL1O + NO ₂ → TOL1OHNO ₂	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O ₃ → OXYL1O ₂	k_C6H50_03	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 → MC3ODBCO ₂ H + 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	TLBIPERNO ₃ + OH → TLOBIPEROH + NO ₂	7.16E-11	Rickard and Pascoe (2009)
G47433	TrGAroC	TLOBIPEROH + OH → C ₅ CO ₁₄ O ₂ + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO ₃ + HO ₂ → C ₆ 15CO ₂ O ₂ + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₂ H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₃ H	KAPH02*rco3_ohh	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO ₃ + NO → C ₆ 15CO ₂ O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO ₃ + NO ₂ → TLEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO ₃ + NO ₃ → C ₆ 15CO ₂ O ₂ + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G47438	TrGAroC	TLEMUCCO3 → C615CO2O2 + CO ₂	k1_R02RCO3	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)*
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_R02sOR02	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_R02RCO3	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_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
G47458	TrGAroC	MCATEC1O + O ₃ → MCATEC1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47459	TrGAroC	TLEMUCCO2H + OH → C615CO2O2 + CO ₂	5.98E-11	Rickard and Pascoe (2009)
G47460	TrGAroC	TLEMUCCO3H + OH → TLEMUCCO3	6.29E-11	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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)
G47470	TrGAroCN	PTLQONE + NO ₃ → NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
G47471	TrGAroC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard and Pascoe (2009)
G47472	TrGAroCN	NCRES1O + NO ₂ → DNCRES	k_C6H5O_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O ₃ → NCRES1O2	k_C6H5O_03	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_C6H5O2_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)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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)
G47497b	TrGAroCN	MNNCATECO2 + HO ₂ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47498	TrGAroCN	MNNCATECO2 + NO → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47499	TrGAroCN	MNNCATECO2 + NO ₃ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47500	TrGAroCN	MNNCATECO2 → NC4MDCO2HN + HCOCO ₂ H + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)
G47501a	TrGAroCN	MNCATECO2 + HO ₂ → MNCATECOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47501b	TrGAroCN	MNCATECO2 + HO ₂ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47502	TrGAroCN	MNCATECO2 + NO → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47503	TrGAroCN	MNCATECO2 + NO ₃ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47504	TrGAroCN	MNCATECO2 → NC4MDCO2HN + HCOCO ₂ H + HO ₂	k1_R02ISOPD02	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	NDNCRESO2 + HO ₂ → NDNCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47509b	TrGAroCN	NDNCRESO2 + HO ₂ → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47510	TrGAroCN	NDNCRESO2 + NO → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47511	TrGAroCN	NDNCRESO2 + NO ₃ → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47512	TrGAroCN	NDNCRESO2 → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G47513a	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{DNCRESOOH}$	$\text{KR02H02}(7) * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G47513b	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{KR02H02}(7) * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G47514	TrGAroCN	$\text{DNCRESO}_2 + \text{NO} \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47515	TrGAroCN	$\text{DNCRESO}_2 + \text{NO}_3 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47516	TrGAroCN	$\text{DNCRESO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47517	TrGAroCN	$\text{NCRES1OOH} + \text{OH} \rightarrow \text{NCRES1O}_2$	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	$\text{MNNCATCOOH} + \text{OH} \rightarrow \text{MNNCATECO}_2$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G47519	TrGAroCN	$\text{MNCATECOOH} + \text{OH} \rightarrow \text{MNCATECO}_2$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G47520	TrGAroC	$\text{C7CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CH}_3\text{C}(\text{O}) + \text{HCOCOCHO}$	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	$\text{C6CO}_2\text{OHCO}_3 + \text{HO}_2 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47521b	TrGAroC	$\text{C6CO}_2\text{OHCO}_3 + \text{HO}_2 \rightarrow \text{C6COOHCO}_3\text{H}$	KAPH02*(rco3_oh+rco3_o3)	Rickard and Pascoe (2009)
G47522	TrGAroCN	$\text{C6CO}_2\text{OHCO}_3 + \text{NO} \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G47523	TrGAroCN	$\text{C6CO}_2\text{OHCO}_3 + \text{NO}_2 \rightarrow \text{C6CO}_2\text{OHPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G47524	TrGAroCN	$\text{C6CO}_2\text{OHCO}_3 + \text{NO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	$\text{C6CO}_2\text{OHCO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G47526	TrGAroCN	$\text{NDNCRESOOH} + \text{OH} \rightarrow \text{NDNCRESO}_2$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G47527	TrGAroCN	$\text{DNCRESOOH} + \text{OH} \rightarrow \text{DNCRESO}_2$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G47528	TrGAroC	$\text{C6COOHCO}_3\text{H} + \text{OH} \rightarrow \text{C6CO}_2\text{OHCO}_3$	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	$\text{C6CO}_2\text{OHPAN} + \text{OH} \rightarrow \text{C5134CO}_2\text{OH} + \text{CO} + \text{CO} + \text{NO}_2$	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	$\text{C6CO}_2\text{OHPAN} \rightarrow \text{C6CO}_2\text{OHCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	$\text{C85O}_2 \rightarrow \text{C86O}_2$	k1_R02tR02	Rickard and Pascoe (2009)
G48201	TrGTerC	$\text{C85O}_2 + \text{HO}_2 \rightarrow \text{C85OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	$\text{C85O}_2 + \text{NO} \rightarrow \text{C86O}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48203	TrGTerC	$\text{C85OOH} + \text{OH} \rightarrow \text{C85O}_2$	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	$\text{C86O}_2 \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3$	k1_R02tR02	Rickard and Pascoe (2009)
G48205	TrGTerCN	$\text{C86O}_2 + \text{NO} \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48206	TrGTerC	$\text{C86O}_2 + \text{HO}_2 \rightarrow \text{C86OOH}$	KR02H02(8)	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G48207	TrGTerC	$C86OOH + OH \rightarrow C86O2$	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	$C811O2 \rightarrow C812O2$	k1_R02pR02	Rickard and Pascoe (2009)
G48209	TrGTerC	$C811O2 + HO_2 \rightarrow 8 \text{ L CARBON}$	KR02H02(8)	Rickard and Pascoe (2009)
G48210	TrGTerCN	$C811O2 + NO \rightarrow C812O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48211	TrGTerC	$C812O2 \rightarrow C813O2$	k1_R02tOR02	Rickard and Pascoe (2009)
G48212	TrGTerCN	$C812O2 + NO \rightarrow C813O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48213	TrGTerC	$C812O2 + HO_2 \rightarrow C812OOH$	KR02H02(8)	Rickard and Pascoe (2009)
G48214	TrGTerC	$C812OOH + OH \rightarrow C812O2$	1.09E-11	Rickard and Pascoe (2009)
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	$C813O2 + HO_2 \rightarrow C813OOH$	KR02H02(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*rc03_ooH	Rickard and Pascoe (2009)
G48221b	TrGTerC	$C721CO3 + HO_2 \rightarrow C721O2 + CO_2 + OH$	KAPH02*rc03_oh	Rickard and Pascoe (2009)
G48221c	TrGTerC	$C721CO3 + HO_2 \rightarrow \text{NORPINIC} + O_3$	KAPH02*rc03_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_CH3C03_NO2	Rickard and Pascoe (2009)
G48224	TrGTerCN	$C721CO3 + NO_3 \rightarrow C721O2 + CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	$C721CO3 \rightarrow C721O2 + CO_2$	k1_R02RC03*0.9	Sander et al. (2019)
G48226	TrGTerC	$C721CO3 \rightarrow \text{NORPINIC}$	k1_R02RC03*0.1	Sander et al. (2019)
G48227	TrGTerC	$C721CO3H + OH \rightarrow C721CO3$	9.65E-12	Rickard and Pascoe (2009)
G48228	TrGTerC	$\text{NORPINIC} + OH \rightarrow C721O2 + CO_2$	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	$C8BCO2 + HO_2 \rightarrow C8BCOOH$	KR02H02(8)	Rickard and Pascoe (2009)
G48233a	TrGTerCN	$C8BCO2 + NO \rightarrow C89O2 + NO_2$	KR02N0*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	$C8BCO2 + NO \rightarrow C8BCNO3$	KR02N0*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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G48237	TrGTerC	$C_8BCCO + OH \rightarrow C_89O_2$	$3.94E-12$	Rickard and Pascoe (2009)
G48238	TrGTerC	$C_89O_2 + HO_2 \rightarrow C_89OOH$	$KR02H02(8)$	Rickard and Pascoe (2009)
G48239a	TrGTerCN	$C_89O_2 + NO \rightarrow C_810O_2 + NO_2$	$KR02N0*(1.-alpha_AN(7,2,0,0,0,$ $temp, cair))$	Rickard and Pascoe (2009)
G48239b	TrGTerCN	$C_89O_2 + NO \rightarrow C_89NO_3$	$KR02N0*alpha_AN(7,2,0,0,0,temp,$ $cair)$	Rickard and Pascoe (2009)
G48240	TrGTerCN	$C_89O_2 + NO_3 \rightarrow C_810O_2 + NO_2$	$KR02N0_3$	Rickard and Pascoe (2009)
G48241	TrGTerC	$C_89O_2 \rightarrow C_810O_2$	$k1_R02tR02$	Rickard and Pascoe (2009)
G48242	TrGTerC	$C_89OOH + OH \rightarrow C_89O_2$	$3.61E-11$	Rickard and Pascoe (2009)
G48243	TrGTerCN	$C_89NO_3 + OH \rightarrow CH_3COCH_3 + CO13C4CHO + NO_2$	$2.56E-11$	Rickard and Pascoe (2009)
G48244	TrGTerC	$C_810O_2 + HO_2 \rightarrow C_810OOH$	$KR02H02(8)$	Rickard and Pascoe (2009)
G48245a	TrGTerCN	$C_810O_2 + NO \rightarrow CH_3COCH_3 + C_514O_2 + NO_2$	$KR02N0*(1.-alpha_AN(10,3,0,0,0,$ $temp, cair))$	Rickard and Pascoe (2009)
G48245b	TrGTerCN	$C_810O_2 + NO \rightarrow C_810NO_3$	$KR02N0*alpha_AN(10,3,0,0,0,$ $temp, cair)$	Rickard and Pascoe (2009)
G48246	TrGTerCN	$C_810O_2 + NO_3 \rightarrow CH_3COCH_3 + C_514O_2 + NO_2$	$KR02N0_3$	Rickard and Pascoe (2009)
G48247	TrGTerC	$C_810O_2 \rightarrow CH_3COCH_3 + C_514O_2$	$k1_R02tR02$	Rickard and Pascoe (2009)
G48248	TrGTerC	$C_810OOH + OH \rightarrow C_810O_2$	$8.35E-11$	Rickard and Pascoe (2009)
G48249	TrGTerCN	$C_810NO_3 + OH \rightarrow CH_3COCH_3 + CO13C4CHO + NO_2$	$4.96E-11$	Rickard and Pascoe (2009)
G48400a	TrGAroC	$LXYL + OH \rightarrow TLEPOXMUC + HO_2 + LCARBON$	$0.401E-11$	Rickard and Pascoe (2009)*
G48400b	TrGAroC	$LXYL + OH \rightarrow C_6H_5CH_2O_2 + LCARBON$	$0.101E-11$	Rickard and Pascoe (2009)*
G48400c	TrGAroC	$LXYL + OH \rightarrow CRESOL + LCARBON$	$0.261E-11$	Rickard and Pascoe (2009)*
G48400d	TrGAroC	$LXYL + OH \rightarrow TLBIPERO_2 + HO_2 + LCARBON$	$0.932E-11$	Rickard and Pascoe (2009)*
G48401	TrGAroCN	$LXYL + NO_3 \rightarrow C_6H_5CH_2O_2 + HNO_3 + LCARBON$	$3.9E-16$	Rickard and Pascoe (2009)*
G48402	TrGAroC	$EBENZ + OH \rightarrow .10 TLEPOXMUC + .07 C_6H_5CH_2O_2 +$ $.18 CRESOL + .65 TLBIPERO_2 + .28 HO_2 + LCARBON$	$7.00E-12$	Rickard and Pascoe (2009)*
G48403	TrGAroCN	$EBENZ + NO_3 \rightarrow C_6H_5CH_2O_2 + HNO_3 + LCARBON$	$1.20E-16$	Rickard and Pascoe (2009)*
G48404	TrGAroCN	$STYRENE + NO_3 \rightarrow NSTYRENO_2$	$1.50E-12$	Rickard and Pascoe (2009)
G48405	TrGAroC	$STYRENE + O_3 \rightarrow .545 HCHO + .1 BENZENE + .28$ $C_6H_5O_2 + .56 CO + .36 OH + .28 HO_2 + .075 PHCOOH$ $+ .545 BENZAL + .09 H_2O_2 + .075 HCOOH + .2 CO_2$	$1.70E-17$	Rickard and Pascoe (2009)*
G48406	TrGAroC	$STYRENE + OH \rightarrow STYRENO_2$	$5.80E-11$	Rickard and Pascoe (2009)
G48407	TrGAroCN	$NSTYRENO_2 + HO_2 \rightarrow NSTYRENOOH$	$KR02H02(8)$	Rickard and Pascoe (2009)
G48408	TrGAroCN	$NSTYRENO_2 + NO \rightarrow NO_2 + NO_2 + HCHO + BENZAL$	$KR02N0$	Rickard and Pascoe (2009)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G48409	TrGAroCN	NSTYRENO2 + NO ₃ → NO ₂ + NO ₂ + HCHO + BENZAL	KR02N03	Rickard and Pascoe (2009)*
G48410	TrGAroCN	NSTYRENO2 → NO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
G48411	TrGAroCN	NSTYRENOOH + OH → NSTYRENO2	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	STYRENO2 + HO ₂ → STYRENOOH	KR02H02(8)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G48412b	TrGAroC	STYRENO2 + HO ₂ → HO ₂ + OH + HCHO + BENZAL	KR02H02(8)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G48413	TrGAroCN	STYRENO2 + NO → NO ₂ + HO ₂ + HCHO + BENZAL	KR02N0	Rickard and Pascoe (2009)*
G48414	TrGAroCN	STYRENO2 + NO ₃ → NO ₂ + HO ₂ + HCHO + BENZAL	KR02N03	Rickard and Pascoe (2009)*
G48415	TrGAroC	STYRENO2 → HO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
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), Sander et al. (2019)
G49208b	TrGTerC	C97O2 + HO ₂ → C98O2 + OH	KR02H02(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G49209	TrGTerC	C97OOH + OH → C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 → C614O2 + CH 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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G49216	TrGTerC	$C85CO3 \rightarrow C85O2 + CO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G49217	TrGTerCN	$C85CO3 + NO \rightarrow C85O2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G49218	TrGTerCN	$C85CO3 + NO_2 \rightarrow C9PAN2$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G49219a	TrGTerC	$C85CO3 + HO_2 \rightarrow C85CO3H$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G49219b	TrGTerC	$C85CO3 + HO_2 \rightarrow C85O2 + CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G49220	TrGTerCN	$C9PAN2 \rightarrow C85CO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G49221	TrGTerCN	$C9PAN2 + OH \rightarrow C85OOH + CO + NO_2$	6.60E-12	Rickard and Pascoe (2009)
G49222	TrGTerC	$C85CO3H + OH \rightarrow C85CO3$	1.02E-11	Rickard and Pascoe (2009)
G49223a	TrGTerC	$C89CO3 \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2$	k1_R02RC03*0.9	Sander et al. (2019)
G49223b	TrGTerC	$C89CO3 \rightarrow C89CO2H$	k1_R02RC03*0.1	Sander et al. (2019)
G49224a	TrGTerC	$C89CO3 + HO_2 \rightarrow C89CO3H$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G49224b	TrGTerC	$C89CO3 + HO_2 \rightarrow C89CO2H + O_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G49224c	TrGTerC	$C89CO3 + HO_2 \rightarrow .80 C811CO3 + .20 C89O2 + .2 CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G49225	TrGTerCN	$C89CO3 + NO_2 \rightarrow C89PAN$	k_CH3C03_NO2	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	Sander et al. (2019)
G49231b	TrGTerC	$C811CO3 \rightarrow PINIC$	k1_R02RC03*0.1	Sander et al. (2019)
G49232a	TrGTerC	$C811CO3 + HO_2 \rightarrow C811CO3H$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G49232b	TrGTerC	$C811CO3 + HO_2 \rightarrow PINIC + O_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G49232c	TrGTerC	$C811CO3 + HO_2 \rightarrow C811O2 + CO_2 + OH$	KAPH02*rco3_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_NO2	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)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	$\text{KR02H02(9)*rcoch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2019)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G49239	TrGTerC	$\text{NOPINDO2} \rightarrow \text{C89CO3}$	k1_R02pOR02	Rickard and Pascoe (2009)
G49240	TrGTerC	$\text{NOPINDOOH} \rightarrow \text{NOPINDCO}$	2.63E-11	Rickard and Pascoe (2009)
G49241	TrGTerC	$\text{NOPINDCO} + \text{OH} \rightarrow \text{C89CO3}$	3.07E-12	Rickard and Pascoe (2009)
G49242	TrGTerC	$\text{NOPINOO} \rightarrow \text{NOPINONE} + \text{H}_2\text{O}_2$	$6.00\text{E-}18*\text{c}(\text{ind_H2O})$	Rickard and Pascoe (2009)
G49243	TrGTerC	$\text{NOPINOO} + \text{CO} \rightarrow \text{NOPINONE} + \text{CO}_2$	1.2E-15	Rickard and Pascoe (2009)
G49244	TrGTerCN	$\text{NOPINOO} + \text{NO} \rightarrow \text{NOPINONE} + \text{NO}_2$	1.E-14	Rickard and Pascoe (2009)
G49245	TrGTerCN	$\text{NOPINOO} + \text{NO}_2 \rightarrow \text{NOPINONE} + \text{NO}_3$	1.E-15	Rickard and Pascoe (2009)
G49246	TrGTerC	$\text{NORPINENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C86O2}$	$\text{k_CH2CHOH_OH_HCOOH}$	Sander et al. (2019), So et al. (2014)*
G49247	TrGTerC	$\text{NORPINENOL} + \text{HCOOH} \rightarrow \text{NORPINAL} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G49248	TrGTerC	$\text{NORPINAL} + \text{HCOOH} \rightarrow \text{NORPINENOL} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G49249	TrGTerC	$\text{C811CO3H} + \text{OH} \rightarrow \text{C811CO3}$	1.04E-11	Rickard and Pascoe (2009)
G49250	TrGTerCN	$\text{C811PAN} \rightarrow \text{C811CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	$\text{C811PAN} + \text{OH} \rightarrow \text{C721CHO} + \text{CO} + \text{NO}_2$	6.77E-12	Rickard and Pascoe (2009)
G49400a	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + 2 \text{LCARBON}$	0.827E-11	Rickard and Pascoe (2009)*
G49400b	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{C6H5CH2O2} + 2 \text{LCARBON}$	0.189E-11	Rickard and Pascoe (2009)*
G49400c	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{CRESOL} + 2 \text{LCARBON}$	0.141E-11	Rickard and Pascoe (2009)*
G49400d	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{TLBIPERO2} + \text{HO}_2 + 2 \text{LCARBON}$	2.917E-11	Rickard and Pascoe (2009)*
G49401	TrGAroCN	$\text{LTMB} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + 2 \text{LCARBON}$	1.52E-15	Rickard and Pascoe (2009)*
G40200	TrGTerC	$\text{APINENE} + \text{OH} \rightarrow .75 \text{LAPINABO2} + .15 \text{MENTHEN6ONE} + .15 \text{HO}_2 + .10 \text{ROO6R1O2}$	$1.2\text{E-}11*\text{EXP}(440./\text{TEMP})$	Atkinson et al. (2006)*
G40201a	TrGTerCN	$\text{LAPINABO2} + \text{NO} \rightarrow \text{PINAL} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1-(.65*\alpha_{\text{AN}}(11,3,0,0,0,\text{temp},\text{cair})+.35*\alpha_{\text{AN}}(11,2,0,0,0,\text{temp},\text{cair})))$	Rickard and Pascoe (2009), Sander et al. (2019)
G40201b	TrGTerCN	$\text{LAPINABO2} + \text{NO} \rightarrow \text{LAPINABNO3}$	$\text{KR02N0}*(.65*\alpha_{\text{AN}}(11,3,0,0,0,0,\text{temp},\text{cair})+.35*\alpha_{\text{AN}}(11,2,0,0,0,\text{temp},\text{cair})))$	Rickard and Pascoe (2009), Sander et al. (2019)
G40202a	TrGTerC	$\text{LAPINABO2} + \text{HO}_2 \rightarrow \text{LAPINABOOH}$	$\text{KR02H02(10)}*(1-\text{rchohch2o2_oh})$	Rickard and Pascoe (2009), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G40202b	TrGTerC	LAPINABO2 + HO ₂ → PINAL + HO ₂ + OH	KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
G40203	TrGTerC	LAPINABO2 → PINAL + HO ₂	R02*(0.65*k1_R02t0R02+.35*k1_R02s0R02)	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	KR02NO	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO ₂ → 2OHMENTHEN6ONE	KR02H02(10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 → 2OHMENTHEN6ONE + HO ₂	k1_R02t0R02	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH → 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH → .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./TEMP)	Wallington et al. (2018)*
G40212	TrGTerCN	PINAL + NO ₃ → C96CO3 + HNO ₃	2.0E-14	Wallington et al. (2018)*
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*rc03_ooh	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO ₂ → PINONIC + O ₃	KAPH02*rc03_o3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO ₂ → C96O2 + OH + CO ₂	KAPH02*rc03_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	KR02NO3*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	KR02NO*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40223b	TrGTerCN	PINALO2 + NO → PINALNO3	KR02NO*alpha_AN(12,3,0,1,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
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)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G40227	TrGTerC	$C106O2 + HO_2 \rightarrow C106OOH$	KR02H02(10)	Rickard and Pascoe (2009)
G40228a	TrGTerCN	$C106O2 + NO \rightarrow C716O2 + CH_3COCH_3 + NO_2$	$KR02N0*0.875*(1.-\alpha_{AN}(13,3,0,0,0,temp,cair))$	Rickard and Pascoe (2009), Sander et al. (2019)
G40228b	TrGTerCN	$C106O2 + NO \rightarrow C106NO3$	$KR02N0*0.875*\alpha_{AN}(13,3,0,0,0,temp,cair)$	Rickard and Pascoe (2009), Sander et al. (2019)
G40229	TrGTerC	$C106O2 \rightarrow C716O2 + CH_3COCH_3$	k1_R02tR02	Rickard and Pascoe (2009)
G40230	TrGTerC	$C106OOH + OH \rightarrow C106O2$	8.01E-11	Rickard and Pascoe (2009)
G40231	TrGTerCN	$C106NO3 + OH \rightarrow CO235C6CHO + CH_3COCH_3 + NO_2$	7.03E-11	Rickard and Pascoe (2009)
G40232	TrGTerC	$APINENE + O_3 \rightarrow .09 APINBOO + .08 PINONIC + .77 OH + .33 NORPINAL + .33 CO + .33 HO_2 + .06 APINA00 + .44 C109O2$	$8.05E-16*EXP(-640./TEMP)$	Wallington et al. (2018)*
G40233	TrGTerC	$APINA00 \rightarrow PINAL + H_2O_2$	$1.00E-17*c(ind_H20)$	Rickard and Pascoe (2009)
G40234	TrGTerC	$APINA00 + CO \rightarrow PINAL + CO_2$	1.20E-15	Rickard and Pascoe (2009)
G40235	TrGTerCN	$APINA00 + NO \rightarrow PINAL + NO_2$	1.00E-14	Rickard and Pascoe (2009)
G40236	TrGTerCN	$APINA00 + NO_2 \rightarrow PINAL + NO_3$	1.00E-15	Rickard and Pascoe (2009)
G40237a	TrGTerC	$APINBOO \rightarrow PINONIC$	$1.00E-17*c(ind_H20)*(0.08+0.15)$	Rickard and Pascoe (2009)
G40237b	TrGTerC	$APINBOO \rightarrow PINAL + H_2O_2$	$1.00E-17*c(ind_H20)*0.77$	Rickard and Pascoe (2009)
G40238	TrGTerC	$APINBOO + CO \rightarrow PINAL + CO_2$	1.20E-15	Rickard and Pascoe (2009)
G40239	TrGTerCN	$APINBOO + NO \rightarrow PINAL + NO_2$	1.00E-14	Rickard and Pascoe (2009)
G40240	TrGTerCN	$APINBOO + NO_2 \rightarrow PINAL + NO_3$	1.00E-15	Rickard and Pascoe (2009)
G40241	TrGTerC	$C109O2 \rightarrow C89CO3 + HCHO$	k1_R02pOR02	Rickard and Pascoe (2009)
G40242	TrGTerCN	$C109O2 + NO \rightarrow C89CO3 + HCHO + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G40243a	TrGTerC	$C109O2 + HO_2 \rightarrow C109OOH$	$KR02H02(10)*rcoch2o2_ooH$	Rickard and Pascoe (2009), Sander et al. (2019)
G40243b	TrGTerC	$C109O2 + HO_2 \rightarrow C89CO3 + HCHO + OH$	$KR02H02(10)*rcoch2o2_oh$	Rickard and Pascoe (2009), Sander et al. (2019)
G40244	TrGTerC	$C109OOH + OH \rightarrow C109CO + OH$	5.47E-11	Rickard and Pascoe (2009)
G40245	TrGTerC	$C109CO + OH \rightarrow C89CO3 + CO$	5.47E-11	Rickard and Pascoe (2009)
G40246	TrGTerCN	$APINENE + NO_3 \rightarrow LNAPINABO2$	$1.2E-12*EXP(490./temp)$	Wallington et al. (2018)*
G40247	TrGTerCN	$LNAPINABO2 \rightarrow PINAL + NO_2$	$(0.65*k1_R02tR02 + 0.35*k1_R02sR02)$	Rickard and Pascoe (2009)
G40248	TrGTerCN	$LNAPINABO2 + NO \rightarrow PINAL + NO_2 + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G40249	TrGTerCN	$LNAPINABO2 + HO_2 \rightarrow LNAPINABOOH$	KR02H02(10)	Rickard and Pascoe (2009)
G40250	TrGTerCN	$LNAPINABO2 + NO_3 \rightarrow PINAL + NO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)
G40251	TrGTerCN	$LNAPINABOOH + OH \rightarrow LNAPINABO2$	$(.65*6.87E-12+.35*1.23E-11)$	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
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), Sander et al. (2019)
G40253b	TrGTerC	BPINAO2 + HO ₂ → NOPINONE + HCHO + HO ₂ + OH	KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2019)
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), Sander et al. (2019)
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KR02N0*alpha_AN(11,3,0,0,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO ₂	k1_R02tOR02	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	KR02N0*(1.-alpha_AN(13,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO → ROO6R1NO3	KR02N0*alpha_AN(13,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40259	TrGTerC	ROO6R1O2 + HO ₂ → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40260	TrGTerC	ROO6R1O2 → ROO6R3O2 + CH ₃ COCH ₃	k1_R02tOR02	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO → RO6R3O2 + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO → RO6R1NO3	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO ₂ → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 → RO6R3O2	k1_R02sOR02	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO → 9 LCARBON + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40264b	TrGTerCN	RO6R3O2 + NO → 10 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO ₂ → 10 LCARBON	KR02H02(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)	Wallington et al. (2018)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G40267b	TrGTerC	BPINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267c	TrGTerC	BPINENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267d	TrGTerC	BPINENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40268	TrGTerCN	BPINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40269	TrGTerCN	LNBPINABO2 + HO ₂ → LNBPINABOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40270	TrGTerCN	LNBPINABO2 + NO → NOPINONE + HCHO + NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G40271	TrGTerCN	LNBPINABO2 + NO ₃ → NOPINONE + HCHO + NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G40272a	TrGTerCN	LNBPINABO2 → NOPINONE + HCHO + NO ₂	k1_R02tR02*0.7	Rickard and Pascoe (2009)
G40272b	TrGTerCN	LNBPINABO2 → BPINAN03	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	Sander et al. (2019), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH → PINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G40278	TrGTerC	PINAL + HCOOH → PINEOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G40279a	TrGC	CARENE + OH → LAPINABO2	8.7E-11*(.50+.25)	Wolfe et al. (2011), Sander et al. (2019)
G40279b	TrGC	CARENE + OH → MENTHEN6ONE + HO ₂	8.7E-11*.25*.60	Wolfe et al. (2011), Sander et al. (2019)
G40279c	TrGC	CARENE + OH → ROO6R1O2	8.7E-11*.25*.40	Wolfe et al. (2011), Sander et al. (2019)
G40280a	TrGC	CARENE + O ₃ → APINBOO	2.E-16*.50*.18	Wolfe et al. (2011), Sander et al. (2019)
G40280b	TrGC	CARENE + O ₃ → PINONIC	2.E-16*.50*.16	Wolfe et al. (2011), Sander et al. (2019)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G40280c	TrGC	CARENE + O ₃ → OH + NORPINAL + CO + HO ₂	2.E-16*.50*.66	Wolfe et al. (2011), Sander et al. (2019)
G40280d	TrGC	CARENE + O ₃ → APINAOO	2.E-16*.50*.12	Wolfe et al. (2011), Sander et al. (2019)
G40280e	TrGC	CARENE + O ₃ → OH + C109O2	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Sander et al. (2019)
G40281	TrGCN	CARENE + NO ₃ → LNAPINABO2	9.5E-12	Wolfe et al. (2011), Sander et al. (2019)
G40282a	TrGTerC	SABINENE + OH → BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40282b	TrGTerC	SABINENE + OH → ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40283a	TrGTerC	SABINENE + O ₃ → NOPINONE + .63 CO + .37 HOCH ₂ OOH + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	Wallington et al. (2018)*
G40283b	TrGTerC	SABINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283c	TrGTerC	SABINENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283d	TrGTerC	SABINENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40284	TrGTerCN	SABINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
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)	Wallington et al. (2018)*
G40286b	TrGTerC	CAMPHENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286c	TrGTerC	CAMPHENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286d	TrGTerC	CAMPHENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40287	TrGTerCN	CAMPHENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G40400	TrGAroC	LHAROM + OH → .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + .18 HO ₂ + 4 LCARBON	5.67E-11	Rickard and Pascoe (2009)*
G40401	TrGAroCN	LHAROM + NO ₃ → C6H5CH2O2 + HNO ₃ + 4 LCARBON	2.60E-15	Rickard and Pascoe (2009)*
G6100	UpStTrGCl	Cl + O ₃ → ClO + O ₂	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + O(³ P) → Cl + O ₂	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl ₂ + O ₂	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O ₂	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OCIO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl ₂ O ₂	k_ClO_ClO	Burkholder et al. (2015)
G6103	StTrGCl	Cl ₂ O ₂ → ClO + ClO	k_ClO_ClO/(2.16E-27*EXP(8537./ temp))	Burkholder et al. (2015)*
G6200	StGCl	Cl + H ₂ → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO ₂ → HCl + O ₂	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO ₂ → ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H ₂ O ₂ → HCl + HO ₂	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → .94 Cl + .94 HO ₂ + .06 HCl + .06 O ₂	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO ₂ → HOCl + O ₂	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH → Cl + H ₂ O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH → ClO + H ₂ O	3.0E-12*EXP(-500./temp)	Burkholder et al. (2015)
G6300	UpStTrGCIN	ClO + NO → NO ₂ + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGCIN	ClO + NO ₂ → ClNO ₃	k_3rd_iupac(temp, cair, 1.6E-31, 3.4, 7.E-11, 0., 0.4)	Atkinson et al. (2007)
G6302	TrGCIN	ClNO ₃ → ClO + NO ₂	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGCIN	ClNO ₃ + O(³ P) → ClO + NO ₃	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGCIN	ClNO ₃ + Cl → Cl ₂ + NO ₃	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH ₄ → HCl + CH ₃	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO ₂	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH ₃ OOH → HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH ₃ O ₂ → HO ₂ + Cl + HCHO	1.8E-12*EXP(-600./temp)	Burkholder et al. (2015)
G6404	StGCl	CCl ₄ + O(¹ D) → LCARBON + ClO + 3 Cl	3.3E-10	Burkholder et al. (2015)
G6405	StGCl	CH ₃ Cl + O(¹ D) → 0.1 CH ₃ Cl + 0.1 O(³ P) + 0.46 ClO + 0.35 Cl + 0.09 H + 0.9 LCARBON + 0.09 LCHLORINE	1.65E-10	Burkholder et al. (2015)
G6406	StGCl	CH ₃ Cl + OH → LCARBON + H ₂ O + Cl	1.96E-12*EXP(-1200./temp)	Burkholder et al. (2015)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 2 \text{LCARBON} + \text{OH} + 3 \text{Cl}$	3.25E-10	Burkholder et al. (2015)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 2 \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E-}12 * \text{EXP}(-1520./\text{temp})$	Burkholder et al. (2015)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$k_3\text{rd_iupac}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})$	8.0e-11	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{LCARBON} + \text{CH}_3 + \text{HCl}$	$k_3\text{rd_iupac}(\text{temp}, \text{cair}, 6.1\text{e-}30, 3.0, 2.0\text{e-}10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$8.3\text{E-}11 * \text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
G6413	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{HCl} + \text{HCHO} + \text{NO}_2$	$1.3\text{E-}11 * \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6414	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO} \rightarrow \text{HCl} + \text{HCHO} + \text{NO}$	2.1E-12	Sokolov et al. (1999)
G6415	StTrGCl	$\text{Cl} + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ClO} + .5 \text{CH}_3\text{O} + .5 \text{HCl} + .5 \text{CH}_2\text{OO}$	1.6E-10	Burkholder et al. (2015)
G6416	TrGCCIN	$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{NCCH}_2\text{O}_2 + \text{HCl}$	$1.6\text{E-}11 * \text{EXP}(-2104./\text{temp})$	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019)
G6500	StGCIF	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + 2 \text{LFLUORINE} + \text{ClO} + \text{Cl}$	1.4E-10	Burkholder et al. (2015)
G6501	StGCIF	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + \text{LFLUORINE} + \text{ClO} + 2 \text{Cl}$	2.3E-10	Burkholder et al. (2015)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E-}11 * \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E-}11 * \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14 * \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E-}12 * \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E-}12 * \text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E-}12 * \text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7203	StGBr	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E-}10 * \text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E-}11 * \text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGBrN	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.7\text{E-}12 * \text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGBrN	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_BrO_NO2 / (5.44\text{E-}9 * \text{EXP}(14192./\text{temp}) * 1.6 * R_gas * \text{temp} / (\text{atm}2\text{Pa} * \text{N}_A))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E-}12 * \text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.6\text{E-}12 * \text{EXP}(-1600./\text{temp})$	Kondo and Benson (1984)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G7402	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{CH}_2\text{OO}$	$2.42\text{E}-14 * \text{EXP}(1617./\text{temp})$	Shallcross et al. (2015)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + \text{Br}$	$1.42\text{E}-12 * \text{EXP}(-1150./\text{temp})$	Burkholder et al. (2015)
G7404	TrGBrC	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HBr}$	$2.8\text{E}-13 * \text{EXP}(224./\text{temp}) / (1. + 1.13\text{E}24 * \text{EXP}(-3200./\text{temp}) / \text{C}(\text{ind}_02))$	Atkinson et al. (2006)*
G7405	TrGBrC	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})$	$1.8\text{e}-11 * \text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7406	TrGBrC	$\text{Br} + \text{C}_2\text{H}_2 \rightarrow \text{LCARBON} + \text{CH}_3\text{O}_2 + \text{HBr}$	$6.35\text{e}-15 * \text{EXP}(440./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Br}$	$9.0\text{E}-13 * \text{EXP}(-360./\text{temp})$	Burkholder et al. (2015)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E}-12 * \text{EXP}(-840./\text{temp})$	Burkholder et al. (2015)*
G7600	TrGBrCl	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	$3.32\text{E}-15$	Manion et al. (2015)
G7601	TrGBrCl	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	$1.10\text{E}-15$	Dolson and Leone (1987)
G7602	TrGBrCl	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E}-10 * \text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$1.6\text{E}-12 * \text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E}-12 * \text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	$5.8\text{E}-13 * \text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGBrCl	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	$1.45\text{E}-11$	Clyne and Cruse (1972)
G7605	TrGBrCl	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{LCARBON} + 2 \text{LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E}-12 * \text{EXP}(-840./\text{temp})$	see note*
G7606	TrGBrCl	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E}-12 * \text{EXP}(-840./\text{temp})$	see note*
G7607	TrGBrCl	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.1\text{E}-12 * \text{EXP}(-880./\text{temp})$	Burkholder et al. (2015)*
G9200a	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{SO}_3 + \text{HO}_2$	$k_3\text{rd}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0., 0.6)$	Sander et al. (2011)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E}-11 * \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E}-13 * \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGCS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	$1.\text{E}-10$	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3$	$1.8\text{E}13 * \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	$3.\text{E}-13$	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5.\text{E}-11$	Barone et al. (1995)
G9408	StTrGS	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	k_CH200_S02	Welz et al. (2012), Stone et al. (2014)*
G9409	TrGTerCS	$\text{NOPINO} + \text{SO}_2 \rightarrow \text{NOPINONE} + \text{H}_2\text{SO}_4$	$7.\text{E}-14$	Rickard and Pascoe (2009)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G9410	TrGTerCS	APINAOO + SO ₂ → PINAL + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009)
G9411	TrGTerCS	APINBOO + SO ₂ → PINAL + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009)
G9412	TrGTerCS	MBOOO + SO ₂ → IBUTALOH + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009)
G9600	TrGCCIS	DMS + Cl → CH ₃ SO ₂ + HCl + HCHO	3.3E-10	Atkinson et al. (2004)
G9700	TrGBrCS	DMS + Br → CH ₃ SO ₂ + HBr + HCHO	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGBrCS	DMS + BrO → DMSO + Br	4.4E-13	Ingham et al. (1999)
G01Diag	StTrG	O ₃ (s) → LO ₃ (s)	k_03s	Roelofs and Lelieveld (1997)
G9100	TrStGS	SO + O ₂ → SO ₂ + O(³ P)	1.25e-13*exp(-2190/temp)	Sander et al. (2011)
G9101	TrStGS	SO + O ₃ → SO ₂ + O ₂	3.4e-12*exp(-1100/temp)	Sander et al. (2011)
G9102	TrStGS	S + O ₂ → SO + O(³ P)	2.3e-12	Sander et al. (2011)
G9201	TrStGS	SH + O ₂ → OH + SO	4.e-19	Sander et al. (2011)
G9202	TrStGS	SO ₃ + H ₂ O → H ₂ SO ₄	8.5e-41*exp(6540./temp)*C(ind_ H2O)	Sander et al. (2003)
G9406	TrStGS	OCS + OH → SH + CO ₂	1.1e-13*exp(-1200./temp)	Sander et al. (2011)
G9407	TrStGS	OCS + O(³ P) → CO + SO	2.1e-11*exp(-2200./temp)	Sander et al. (2011)
G49fPOG2	TrG	LfPOG02 + OH → 1.15 LfSOGsv01	2.00E-11	Tsimpidi et al. (2014)
G49fPOG3	TrG	LfPOG03 + OH → 1.15 LfSOGsv02	2.00E-11	Tsimpidi et al. (2014)
G49fPOG4	TrG	LfPOG04 + OH → 1.15 LfSOGiv03	2.00E-11	Tsimpidi et al. (2014)
G49fPOG5	TrG	LfPOG05 + OH → 1.15 LfSOGiv04	2.00E-11	Tsimpidi et al. (2014)
G49bbPOG2	TrG	LbbPOG02 + OH → 1.15 LbbSOGsv01	2.00E-11	Tsimpidi et al. (2014)
G49bbPOG3	TrG	LbbPOG03 + OH → 1.15 LbbSOGsv02	2.00E-11	Tsimpidi et al. (2014)
G49bbPOG4	TrG	LbbPOG04 + OH → 1.15 LbbSOGiv03	2.00E-11	Tsimpidi et al. (2014)
G49fSOGsv2	TrG	LfSOGsv02 + OH → 1.15 LfSOGsv01	2.00E-11	Tsimpidi et al. (2014)
G49fSOGiv2	TrG	LfSOGiv02 + OH → 1.15 LfSOGiv01	2.00E-11	Tsimpidi et al. (2014)
G49fSOGiv3	TrG	LfSOGiv03 + OH → 1.15 LfSOGiv02	2.00E-11	Tsimpidi et al. (2014)
G49fSOGiv4	TrG	LfSOGiv04 + OH → 1.15 LfSOGiv03	2.00E-11	Tsimpidi et al. (2014)
G49bbSOGsv2	TrG	LbbSOGsv02 + OH → 1.15 LbbSOGsv01	2.00E-11	Tsimpidi et al. (2014)
G49bbSOGiv2	TrG	LbbSOGiv02 + OH → 1.15 LbbSOGiv01	2.00E-11	Tsimpidi et al. (2014)
G49bbSOGiv3	TrG	LbbSOGiv03 + OH → 1.15 LbbSOGiv02	2.00E-11	Tsimpidi et al. (2014)
G49TERP1	TrG	LTERP + OH → 0.0812 LbSOGv01 + 0.0695 LbSOGv02 + 0.2714 LbSOGv03 + 0.4598 LbSOGv04	1.8308E-11*EXP(449.38/temp)	Tsimpidi et al. (2014)
G49TERP2	TrG	LTERP + O ₃ → 0.0812 LbSOGv01 + 0.0695 LbSOGv02 + 0.2714 LbSOGv03 + 0.4598 LbSOGv04	1.0805E-15*EXP(-821.26/temp)	Tsimpidi et al. (2014)
G49TERP1	TrGN	LTERP + NO ₃ → 0.0812 LbSOGv01 + 0.0695 LbSOGv02 + 0.2714 LbSOGv03 + 0.4598 LbSOGv04	3.6616E-12*EXP(174.62/temp)	Tsimpidi et al. (2014)

Table S1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G49TERP1	TrG	LTERP + O(¹ D) → 0.0812 LbSOGv01 + 0.0695 LbSOGv02 + 0.2714 LbSOGv03 + 0.4598 LbSOGv04	3.2714E-11	Tsimpidi et al. (2014)
G49AR01	TrG	LALK4 + OH → 0.0000 LaSOGv01 + 0.0183 LaSOGv02 + 0.0000 LaSOGv03 + 0.0000 LaSOGv04	5.9525902E-12*EXP(-90.58/temp)	Tsimpidi et al. (2014)
G49AR01	TrG	LALK5 + OH → 0.0000 LaSOGv01 + 0.1070 LaSOGv02 + 0.0000 LaSOGv03 + 0.0000 LaSOGv04	1.1104831E-11*EXP(-51.83/temp)	Tsimpidi et al. (2014)
G49AR01	TrG	LOLE2 + OH → 0.0017 LaSOGv01 + 0.0135 LaSOGv02 + 0.0435 LaSOGv03 + 0.1424 LaSOGv04	1.7407701E-11*EXP(384.46/temp)	Tsimpidi et al. (2014)
G49AR01	TrG	LOLE2 + O ₃ → 0.0017 LaSOGv01 + 0.0135 LaSOGv02 + 0.0435 LaSOGv03 + 0.1424 LaSOGv04	5.0221891E-16*EXP(-461.45/temp)	Tsimpidi et al. (2014)
G49AR01	TrGN	LOLE2 + NO ₃ → 0.0017 LaSOGv01 + 0.0135 LaSOGv02 + 0.0435 LaSOGv03 + 0.1424 LaSOGv04	7.2628560E-13*EXP(0.00/temp)	Tsimpidi et al. (2014)
G49AR01	TrG	LOLE2 + O(¹ D) → 0.0017 LaSOGv01 + 0.0135 LaSOGv02 + 0.0435 LaSOGv03 + 0.1424 LaSOGv04	2.0909145E-11	Tsimpidi et al. (2014)
G49aSOGv2	TrG	LaSOGv02 + OH → 1.075 LaOSOGv01	1.00E-11	Tsimpidi et al. (2014)
G49aSOGv3	TrG	LaSOGv03 + OH → 1.075 LaOSOGv02	1.00E-11	Tsimpidi et al. (2014)
G49aSOGv4	TrG	LaSOGv04 + OH → 1.075 LaOSOGv03	1.00E-11	Tsimpidi et al. (2014)
G49aOSOGv2	TrG	LaOSOGv02 + OH → 1.075 LaOSOGv01	1.00E-11	Tsimpidi et al. (2014)
G49aOSOGv3	TrG	LaOSOGv03 + OH → 1.075 LaOSOGv02	1.00E-11	Tsimpidi et al. (2014)

General notes

Three-body reactions

Rate coefficients for three-body reactions are defined via the function $\mathbf{k_3rd}(T, M, k_0^{300}, n, k_{\text{inf}}^{300}, m, f_c)$. 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} , $\mathbf{k_3rd}$ 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 $\mathbf{k_3rd_iupac}$ here, is used by Wallington et al. (2018) for three-body reactions. It has the same function parameters as $\mathbf{k_3rd}$ 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 $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \mathbf{k_CH3O2}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, $\mathbf{k_CH3O2}$ = second-order rate coefficient of the self reaction of CH₃O₂, and [RO₂] = sum of the concentrations of all organic peroxy radicals.

Specific notes

G1002a: The path leading to 2 O(³P) + O₂ results in a null cycle regarding odd oxygen and is neglected.

G2110: The rate coefficient is: $\mathbf{k_H02_H02} = (3.0\text{E-}13 * \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 * \text{EXP}(920./\text{temp}) * \text{cair}) * (1. + 1.4\text{E-}21 * \text{EXP}(2200./\text{temp}) * \text{C}(\text{ind_H2O}))$.

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

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

G3203: The rate coefficient is: $\mathbf{k_NO2_H02} = \mathbf{k_3rd}(\text{temp}, \text{cair}, 1.9\text{E-}31, 3.4, 4.0\text{E-}12, 0.3, 0.6)$.

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

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).

G4109: Same temperature dependence as for CH₃CHO+NO₃ assumed.

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

G4116: Same value as for PAN + OH.

G4126: Same as for G4104 but scaled to match the 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: HOOCH₂OCHO 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 RO₂.

G4148: Same value as for NO₂+CH₃O₂.

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of CH₃O₂NO₂.

G4150: Value for CH₃O₂NO₂ + OH, H-abstraction enhanced by the HO-group by f_{soh}.

G4154: Products assumed to be CH₃O₂ + O₂ (could also be HCHO + O₂ + 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, CH₂OO, 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: $k_{\text{CH3CO3_NO2}} = k_{\text{3rd}}(\text{temp, cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

G42018: The rate coefficient is the same as for the CH₃ channel in G4107 (CH₃OOH+OH).

G42021: The rate coefficient is $k_{\text{PAN_M}} = k_{\text{CH3CO3_NO2}}/9.0\text{E-}29*\text{EXP}(-14000./\text{temp})$, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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

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

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

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

G42047: Orlando et al. (1998) estimated that about 25% of the HOCH₂CH₂O in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + HO₂.

G42051a: Same as for the CH₃O₂ channel in G4107: CH₃OOH+OH.

G42058b: The aldehydic H is assumed to be like the analogous H of HOCH₂CHO.

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

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

G42075: NO₃CH₂CO₂H and NO₃CH₂CO₃H neglected.

G42078: NO₃CH₂CO₂H neglected.

G42082: Same rate constant as for PAN + OH.

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

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

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

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

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

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

G42087: HCOCN is produced but replaced here by its likely oxidation products (HCN + CO₂) as studied by Tyndall et al. (2001b). The rate constant for a typical RO₂ + NO reaction is used.

G42088: NCCH₂OOH is produced but replaced here by its likely oxidation products (HCN + CO₂) as studied by Tyndall et al. (2001b). The rate constant for a typical RO₂ + HO₂ 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 RO₂ + HO₂ reaction from Atkinson (1997) is used here.

G43008: The value for the generic RO₂ + HO₂ reaction from Atkinson (1997) is used here.

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

G43015a: The same value as for G4107 (CH₃OOH + OH) is used, multiplied by the branching ratio of the CH₃O₂ 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 ($n\text{C}_4\text{H}_9\text{O}_2:\text{sC}_4\text{H}_9\text{O}_2$ 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: $\text{sC}_4\text{H}_9\text{O}_2$ products are substituted with 0.636 $\text{MEK} + \text{HO}_2$ 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 $\text{sC}_4\text{H}_9\text{O}_2$.

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 $-\text{OOH}$ group.

G44016: Products assumed to be only from H-abstraction from a secondary C bearing the $-\text{ONO}_2$ group.

G44018: LHMVKABO_2 is $0.12 \text{ HMVKAO}_2 + 0.88 \text{ HMVKBO}_2$.

G44019: LMEKO_2 represents $0.62 \text{ MEKBO}_2 + 0.38 \text{ MEKAO}_2$.

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 ONO_2 group.

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

G44025: Same value as for PAN.

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

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

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

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

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

G44062a: Simplified products.

G44062b: Simplified products.

G44066: Alkyl nitrate formation neglected.

G44070: Alkyl nitrate formation neglected.

G44076: Alkyl nitrate formation neglected.

G44078: Other channel neglected.

G44081: Alkyl nitrate formation neglected.

G44082: Other channel neglected.

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

G44086: Simplified product distribution.

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

G44096: Both LBUT1ENO2 isomers mostly C_2H_5CHO .

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

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

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

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH_3CHOOA products as from $C_3H_6 + O_3$ reaction.

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

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

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

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

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

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

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

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

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

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

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

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

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

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

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

G44139: Simplified oxidation.

G44140: Simplified oxidation.

G44141: Simplified oxidation.

G44142: Simplified oxidation.

G44202: Alkyl nitrate formation neglected.

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

G44205: Alkyl nitrate formation neglected.

G44210: Alkyl nitrate formation neglected.

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

G44402: $KDEC\ NC4DCO_2 \rightarrow MALANHY + NO_2$

G44406c: $KDEC\ MALDIALCO_2 \rightarrow .6\ MALANHY + HO_2 + .4\ GLYOX + .4\ CO + .4\ CO_2$

G44407: $KDEC\ MALDIALCO_2 \rightarrow .6\ MALANHY + HO_2 + .4\ GLYOX + .4\ CO + .4\ CO_2$

G44409: $KDEC\ MALDIALCO_2 \rightarrow .6\ MALANHY + HO_2 + .4\ GLYOX + .4\ CO + .4\ CO_2$

G44410: $KDEC\ MALDIALCO_2 \rightarrow .6\ MALANHY + HO_2 + .4\ GLYOX + .4\ CO + .4\ CO_2$

G44412: $KDEC\ BZFUONOOA \rightarrow .5\ BZFUONOO + .5\ CO + .5\ CO_2 + .5\ HCOCH_2O_2 + .5\ OH$ and $BZFUONOO \rightarrow .625\ CO_{14}O_3CO_2H + .375\ CO_{14}O_3CHO + .375\ H_2O_2$

G44421: Only major channel.

G44424: $KDEC: GLYOOA \rightarrow .125\ HCHO + .18\ GLYOO + 0.82\ HO_2 + .57\ OH + 1.265\ CO + .25\ CO_2$ and H_2O substitution $GLYOO \rightarrow .625\ HCOCO_2H + .375\ GLYOX + .375\ H_2O_2$

G44425: Merged equations.

G44430: $KDEC\ MALANHYO \rightarrow HCOCOHC O_3$

G44431: $KDEC\ MALANHYO \rightarrow HCOCOHC O_3$

G44432: Only major channel. $KDEC\ MALANHYO \rightarrow HCOCOHC O_3$

G44436: $KDEC\ NBZFUO \rightarrow .5\ CO_{14}O_3CHO + .5\ NO_2 + .5\ NBZFUONE + .5\ HO_2$

G44437: $KDEC\ NBZFUO \rightarrow .5\ CO_{14}O_3CHO + .5\ NO_2 + .5\ NBZFUONE + .5\ HO_2$

G44438: $KDEC\ NBZFUO \rightarrow .5\ CO_{14}O_3CHO + .5\ NO_2 + .5\ NBZFUONE + .5\ HO_2$ and RO_2 Only major channel.

G44439: $KDEC\ MALDIALCO_2 \rightarrow .6\ MALANHY + HO_2 + .4\ GLYOX + .4\ CO + .4\ CO_2$

G44443: $KDEC\ MECOACETO \rightarrow CH_3CO_3 + HCHO$

G44444: $KDEC\ MECOACETO \rightarrow CH_3CO_3 + HCHO$

G44445: $KDEC\ MECOACETO \rightarrow CH_3CO_3 + HCHO$

G44450: $KDEC\ BZFUO \rightarrow CO_{14}O_3CHO + HO_2$

G44451: $KDEC\ BZFUO \rightarrow CO_{14}O_3CHO + HO_2$

G44452: $KDEC\ BZFUO \rightarrow CO_{14}O_3CHO + HO_2$. Only major channel.

G44457: $KDEC\ MALDIALO \rightarrow GLYOX + GLYOX + HO_2$

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 ISOP-BOOH and ISOPDOOH.

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

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

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant 4.16E-11.

G45047: Alkyl nitrate formation neglected.

G45055: Alkyl nitrate formation neglected.

G45071: Alkyl nitrate formation neglected.

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

G45080: Alkyl nitrate formation neglected.

G45092a: C4MDIAL = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with 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 CH₃COCHOHCHO 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 (C4MDIAL) 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 by its oxidation product BENZAL.

G47405: Merged.

G47406: Merged.

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

G47408a: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MG-LYOX + HO₂ + .2 C₄MDIAL + .2 C₅DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

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

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

G47410: Only major channel and KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MG-LYOX + 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 → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

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

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

G47423: KDEC NCRESO → C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO → C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

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

G47436: KFPAN →k_CH3CO3_NO2

G47438: Only major channel.

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

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

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

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

G47445: KFPAN →k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

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

G47483: KDEC NPTLQO → C7CO4DB + NO2

G47484: KDEC NPTLQO → C7CO4DB + NO2

G47485: KDEC NPTLQO → C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO → C6CO2OHCO3

G47487: KDEC PTLQO → C6CO2OHCO3

G47488: KDEC PTLQO → C6CO2OHCO3

G47489: Only major channel. KDEC PTLQO → C6CO2OHCO3.

G47494: New channel.

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

G47498: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + NO2

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

G47502: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

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

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

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

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

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

G47514: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G48202: Alkyl nitrate formation neglected.

G48205: Alkyl nitrate formation neglected.

G48210: Alkyl nitrate formation neglected.

G48212: Alkyl nitrate formation neglected.

G48216: Alkyl nitrate formation neglected.

G48222: Alkyl nitrate formation neglected.

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

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

G48400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(1.36E-11*0.16 + 2.31E-11*0.17 + 1.43E-11*0.12)/3$,

where k and coefficients are for the single isomers ortho, meta and para from MCM.

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

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

G48402: merged under same rate constant

G48403: Same products as for toluene

G48405: KDEC CH₂O₂B → .24 CH₂O + .40 CO + .36 HO₂ + .36 CO + .36 OH and H₂O_{sub} PHCHO → .625 PHCOOH + .375 BENZAL + .375 H₂O₂ + .2 CO₂

G48408: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

G48409: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

G48410: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

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

G48413: KDEC STYRENO → HO₂ + HCHO + BENZAL

G48414: KDEC STYRENO → HO₂ + HCHO + BENZAL

G48415: KDEC STYRENO → HO₂ + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

G49246: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂. Instead of the (lacking) carbonyl a product of further degradation is assumed.

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

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

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

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

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

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

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

G40200: Products from Vereecken et al. (2007). 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, $(k_{ads}+k_{adt})*acoch_3 = 6.46E-11$ where $k_{ads} = 3.0E-11$, $k_{adt} = 5.5E-11$, $acoch_3 = 0.76$

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard and Pascoe (2009).

G40212: Products from Rickard and Pascoe (2009).

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

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard and Pascoe (2009).

G40248: Alkyl nitrate formation neglected.

G40252a: Products from Vereecken and Peeters (2012).

G40252b: Products from Vereecken and Peeters (2012).

G40259: ROO₆R₁OOH is produced but no sink for it.

G40262: RO₆R₁OOH is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

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

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for RO₆R₁NO₃ in G4085.

G40276: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G40282a: Products from Vereecken and Peeters (2012).

G40282b: Products from Vereecken and Peeters (2012).

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

G40284: Products from Rickard and Pascoe (2009).

G40285a: Products from Vereecken and Peeters (2012).

G40285b: Products from Vereecken and Peeters (2012).

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

G40287: Products from Rickard and Pascoe (2009).

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

G40401: Same products as for toluene.

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

G6204: At low temperatures, there may be a minor reaction channel leading to O₃+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

G6402: The initial products are probably HCl and CH₂OOH (Atkinson et al., 2006). It is assumed that CH₂OOH dissociates into HCHO and OH.

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

G7302: The rate coefficient is: $k_{\text{BrO}_2} = k_{\text{3rd}}(\text{temp}, \text{cair}, 5.2\text{E}-31, 3.2, 6.9\text{E}-12, 2.9, 0.6)$.

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

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

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

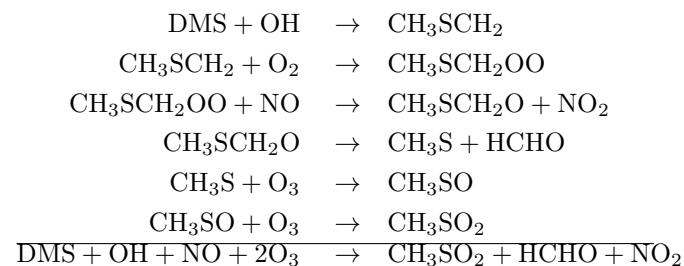
G7408: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7605: Same value as for G7408: CH₂Br₂+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

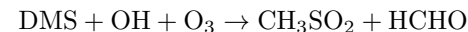
G7606: Same value as for G7408: CH₂Br₂+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

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

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: $k_{\text{DMS}_\text{OH}} = 1.0\text{E}-39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{ind}_02) / (1.+5.0\text{E}-30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{ind}_02))$.

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

Table S2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
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)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	Sander et al. (2014)
J3100	UpStGJN	$N_2O + h\nu \rightarrow O(^1D) + N_2$	jx(ip_N20)	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_N02)	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow N + O(^3P)$	jx(ip_NO)	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_H0NO)	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)
J41002	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	jx(ip_CO2)	Sander et al. (2014)
J41003	StGJ	$CH_4 + h\nu \rightarrow .42 CH_3 + .42 H + .6912 H_2 + .0864 HCHO + .0864 O(^3P) + .1584 OH + .1584 HO_2 + .2112 CO_2 + .1824 CO + .024 H_2O + .10 LCARBON$	jx(ip_CH4)	Sander et al. (2014)*
J41004	StTrGJN	$CH_3ONO + h\nu \rightarrow CH_3O + NO$	jx(ip_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_CH302NO2)	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_CH302NO2)	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)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42002	TrGJC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + h\nu \rightarrow \text{CH}_3 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH3C03H})$	Sander et al. (2014)
J42004	TrGJCN	$\text{PAN} + h\nu \rightarrow .7 \text{CH}_3\text{C}(\text{O}) + .7 \text{NO}_2 + .3 \text{CH}_3 + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2014)*
J42005a	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{HCHO} + 2 \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH2CHO}) * 0.83$	Sander et al. (2014)*
J42005b	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCOCH}_2\text{O}_2$	$\text{jx}(\text{ip_HOCH2CHO}) * 0.07$	Sander et al. (2014)*
J42005c	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{CH}_3\text{OH} + \text{CO}$	$\text{jx}(\text{ip_HOCH2CHO}) * 0.10$	Sander et al. (2014)*
J42006	TrGJC	$\text{HOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J42007	TrGJCN	$\text{PHAN} + h\nu \rightarrow .7 \text{HOCH}_2\text{CO} + .7 \text{NO}_2 + .3 \text{HCHO} + .3 \text{HO}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip_PAN})$	see note*
J42008	TrGJC	$\text{GLYOX} + h\nu \rightarrow 2 \text{CO} + 2 \text{HO}_2$	$\text{jx}(\text{ip_GLYOX})$	Sander et al. (2014)
J42009	TrGJC	$\text{HCOCO}_2\text{H} + h\nu \rightarrow 2 \text{HO}_2 + \text{CO} + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J42010	TrGJC	$\text{HCOCO}_3\text{H} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J42011	TrGJC	$\text{HYETHO}_2\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J42012	TrGJCN	$\text{ETHOHNO}_3 + h\nu \rightarrow \text{HO}_2 + 2 \text{HCHO} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)
J42013	TrGJC	$\text{HOOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	$2 * \text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J42014	TrGC	$\text{HOOCH}_2\text{CO}_2\text{H} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J42015	TrGC	$\text{CH}_2\text{CO} + h\nu \rightarrow .4 \text{CO}_2 + .8 \text{H} + .34 \text{CO} + .34 \text{OH} + .34 \text{HO}_2 + .16 \text{HCHO} + .16 \text{O}({}^3\text{P}) + .1 \text{HCOOH} + \text{CO}$	$\text{J_ketene} * 0.36$	Sander et al. (2019)
J42016	TrGC	$\text{CH}_3\text{CHOHOOH} + h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J42017	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	$(\text{jx}(\text{ip_C2H5N03}) + \text{jx}(\text{ip_CH3CHO})) * (\text{jx}(\text{ip_NOA}) + 1\text{E}-10) / (0.59 * \text{J_IC3H7N03} + \text{jx}(\text{ip_CH3COCH3}) + 1\text{E}-10)$	Sander et al. (2019)*
J42018	TrGJC	$\text{HOOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Sander et al. (2019)
J42019	TrGJCN	$\text{C}_2\text{H}_5\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{jx}(\text{ip_C2H5N03})$	Sander et al. (2019)
J42020	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow .7 \text{NO}_3\text{CH}_2\text{CO}_3 + .7 \text{NO}_2 + .3 \text{HCHO} + .3 \text{NO}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2019)*
J42021	StTrGJCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{C}_2\text{H}_5\text{O}_2 + .333 \text{NO}_3 + .333 \text{CH}_3\text{CHO} + .333 \text{HO}_2$	$\text{jx}(\text{ip_CH302N02})$	Sander et al. (2019)*
J43000	TrGJC	$\text{iC}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43001	TrGJC	$\text{CH}_3\text{COCH}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CH}_3$	$\text{jx}(\text{ip_CH3COCH3})$	Sander et al. (2014)
J43002	TrGJC	$\text{CH}_3\text{COCH}_2\text{OH} + h\nu \rightarrow .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{HO}_2 + .5 \text{HOCH}_2\text{CO} + .5 \text{CH}_3$	J_ACETOL	Sander et al. (2014)*
J43003	TrGJC	$\text{MGLYOX} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2014)
J43004	TrGJC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Rickard and Pascoe (2009)
J43005	TrGJC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Sander et al. (2019)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43006	TrGJCN	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	J_IC3H7N03	von Kuhlmann et al. (2003)*
J43007	TrGJCN	$NOA + h\nu \rightarrow CH_3C(O) + HCHO + NO_2$	jx(ip_NOA)	Barnes et al. (1993)
J43009	TrGJC	$HYPPO_2H + h\nu \rightarrow CH_3CHO + HCHO + HO_2 + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43010	TrGJCN	$PR_2O_2HNO_3 + h\nu \rightarrow NOA + HO_2 + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43011	TrGJC	$HOCH_2COCHO + h\nu \rightarrow HOCH_2CO + CO + HO_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J43012	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HCOCO + HCHO + OH$	jx(ip_CH300H)+J_ACETOL	Sander et al. (2019)
J43013	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HOOCH_2CO_3 + CO + HO_2$	jx(ip_MGLYOX)	Sander et al. (2019)
J43014	TrGJTerC	$HCOCH_2CHO + h\nu \rightarrow HCOCH_2O_2 + HO_2 + CO$	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J43015	TrGJTerC	$HCOCH_2CO_2H + h\nu \rightarrow HCOCH_2O_2 + CO_2 + HO_2$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J43016	TrGJTerC	$HOC_2H_4CO_3H + h\nu \rightarrow HOCH_2CH_2O_2 + CO_2 + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43017	TrGJC	$HCOCOCHO + h\nu \rightarrow HCOCO + HO_2 + CO$	2.*jx(ip_MGLYOX)	Sander et al. (2019)
J43018	TrGJC	$CH_3COCO_2H + h\nu \rightarrow .32 CH_3CHO + .16 CH_2CHOH + .54 CO_2 + .38 CH_3C(O) + .38 HO_2 + .38 CO_2 + .07 CH_3COOH + .07 CO + .05 CH_3C(O) + .05 CO + .05 OH$	JX(IP_CH3COC02H)	Sander et al. (2019)*
J43019	TrGC	$CH_3COCO_3H + h\nu \rightarrow CH_3C(O) + OH + CO_2$	JX(IP_MGLYOX)+jx(ip_CH300H)	Sander et al. (2019)
J43020	TrGC	$CH_3CHCO + h\nu \rightarrow C_2H_4 + CO$	J_ketene*0.36*2.	Sander et al. (2019)
J43021	TrGCN	$PROPOLNO_3 + h\nu \rightarrow HOCH_2CHO + HCHO + HO_2 + NO_2$	J_IC3H7N03	Sander et al. (2019)
J43022	TrGCN	$CH_3COCH_2OONO_2 + h\nu \rightarrow CH_3C(O) + HCHO + NO_3$	jx(ip_CH302N02)+jx(ip_CH3COCH3)	Sander et al. (2019)
J43023	TrGJC	$C_3H_7OOH + h\nu \rightarrow C_2H_5CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J43024	TrGJCN	$C_3H_7ONO_2 + h\nu \rightarrow C_2H_5CHO + NO_2 + HO_2$	0.59*J_IC3H7N03	see note*
J43025a	TrGJC	$C_2H_5CHO + h\nu \rightarrow C_2H_5O_2 + HO_2 + CO$	jx(ip_C2H5CHO2HCO)	see note*
J43025b	TrGJC	$C_2H_5CHO + h\nu \rightarrow CH_2CHCH_2OH$	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Sander et al. (2019)*
J43026	TrGJCN	$PPN + h\nu \rightarrow .7 C_2H_5CO_3 + .7 NO_2 + .3 C_2H_5O_2 + .3 CO_2 + .3 NO_3$	jx(ip_PAN)	Sander et al. (2014)
J43027	TrGJC	$C_2H_5CO_3H + h\nu \rightarrow C_2H_5O_2 + CO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J43028a	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HOOCH_2CO_3 + CO + HO_2$	jx(ip_MGLYOX)	Sander et al. (2019)
J43028b	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HCOCO + HCHO + OH$	jx(ip_HOCH2CHO)+jx(ip_CH300H)	Sander et al. (2019)
J43200	TrGJTerC	$HCOCH_2CO_3H + h\nu \rightarrow HCOCH_2O_2 + CO_2 + OH$	jx(ip_HOCH2CHO)+jx(ip_CH300H)	Rickard and Pascoe (2009)
J43400	TrGJAroC	$C_3DIALOOH + h\nu \rightarrow GLYOX + CO + HO_2 + OH$	jx(ip_HOCH2CHO)*2+jx(ip_CH300H)	Rickard and Pascoe (2009)*
J43401	TrGJAroC	$C_3_2OH_13CO + h\nu \rightarrow GLYOX + HO_2 + HO_2 + CO$	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J43402	TrGJAroC	$HCOCOHC_3H + h\nu \rightarrow GLYOX + HO_2 + CO_2 + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44000a	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_p}/(\text{k_p}+\text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2019)
J44000b	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_s}/(\text{k_p}+\text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2019)
J44001	TrGJC	$\text{MVK} + h\nu \rightarrow .5 \text{ C}_3\text{H}_6 + .5 \text{ CH}_3\text{C}(\text{O}) + .5 \text{ HCHO} + \text{CO} + .5 \text{ HO}_2$	$\text{jx}(\text{ip_MVK})$	Sander et al. (2014)
J44002	TrGJC	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$	$0.42 * \text{jx}(\text{ip_CHOH})$	von Kuhlmann et al. (2003)
J44003	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow .62 \text{ CH}_3\text{C}(\text{O}) + .62 \text{ CH}_3\text{CHO} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 0.42 * \text{jx}(\text{ip_CHOH})$	Sander et al. (2019)
J44004	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{ CH}_3\text{C}(\text{O})$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	see note*
J44005a	TrGJCN	$\text{LC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{J_IC3H7N03} * (\text{k_p}/(\text{k_p}+\text{k_s}))$	see note*
J44005b	TrGJCN	$\text{LC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$	$\text{J_IC3H7N03} * (\text{k_s}/(\text{k_p}+\text{k_s}))$	see note*
J44006	TrGJCN	$\text{MPAN} + h\nu \rightarrow .7 \text{ MACO}_3 + .7 \text{ NO}_2 + .3 \text{ MACO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	see note*
J44007a	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H})$	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	$\text{MACR} + h\nu \rightarrow .5 \text{ MACO}_3 + .5 \text{ CH}_3\text{C}(\text{O}) + .5 \text{ HCHO} + .5 \text{ CO} + \text{HO}_2$	$\text{jx}(\text{ip_MACR})$	Sander et al. (2014)
J44009	TrGJC	$\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)*
J44010	TrGJC	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$	see note*
J44011	TrGJC	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44012	TrGJC	$\text{LHMVKABOOH} + h\nu \rightarrow .12 \text{ MGLYOX} + .12 \text{ HO}_2 + .88 \text{ CH}_3\text{C}(\text{O}) + .88 \text{ HOCH}_2\text{CHO} + .12 \text{ HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Sander et al. (2019)
J44013	TrGJC	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{J_ACETOL}$	Sander et al. (2019)
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	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	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	Sander et al. (2019)
J44017a	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{ CH}_3\text{COCO}_2\text{H} + .1848 \text{ H}_2\text{O}_2 + .2208 \text{ MGLYOX} + .36 \text{ OH} + .36 \text{ CO} + .56 \text{ CH}_3\text{C}(\text{O}) + .2 \text{ CH}_3\text{CHO} + .2 \text{ CO}_2 + .2 \text{ HCHO} + .2 \text{ HO}_2 + \text{CO}$	$\text{J_KETENE} * 0.5$	Sander et al. (2019), Rickard and Pascoe (2009)*
J44017b	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$	$\text{J_KETENE} * 0.5$	Sander et al. (2019)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44018a	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J44018b	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J44019	TrGJC	$\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$	$3.15 * \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J44020a	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Rickard and Pascoe (2009)
J44020b	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J44021	TrGJTerC	$\text{C44OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J44022	TrGJTerC	$\text{C413COOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{J_ACETOL}$	Rickard and Pascoe (2009)
J44023a	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J44023b	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J44024	TrGJTerC	$\text{C312COCO}_3\text{H} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J44025	TrGJCN	$\text{LMEKNO}_3 + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{jx}(\text{ip_MEKNO}_3)$	Barnes et al. (1993), Sander et al. (2019)*
J44026	TrGJCN	$\text{MVKNO}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{NO}_2$	$\text{jx}(\text{ip_MEKNO}_3)$	Barnes et al. (1993), Sander et al. (2019)*
J44027	TrGJCN	$\text{MACRN} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$(2.84 * \text{J_IC3H7NO}_3 + \text{jx}(\text{ip_CH}_3\text{CHO})) * (\text{jx}(\text{ip_MEKNO}_3) + 1\text{E}-10) / (\text{J_IC3H7NO}_3 + 0.42 * \text{jx}(\text{ip_CHOH}) + 1\text{E}-10)$	Müller et al. (2014), Sander et al. (2019)*
J44028	TrGJCN	$\text{TC4H9NO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{NO}_2$	$2.84 * \text{J_IC3H7NO}_3$	Sander et al. (2019)
J44029	TrGJC	$\text{TC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44030	TrGJCN	$\text{IBUTOLBNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{J_IC3H7NO}_3$	Sander et al. (2019)
J44031	TrGJC	$\text{IBUTOLBOOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44032	TrGJC	$\text{LBUT1ENOOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44033	TrGJCN	$\text{LBUT1ENNO}_3 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7NO_3	Sander et al. (2019)
J44034	TrGJC	$\text{BUT2OLOOH} + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44035	TrGJCN	$\text{BUT2OLNO}_3 + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7NO_3	Sander et al. (2019)
J44036	TrGJC	$\text{BUT2OLO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	J_ACETOL	Sander et al. (2019)
J44037a	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_C3H7CHO2HCO})$	Sander et al. (2019)
J44037b	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{CHOH}$	$\text{jx}(\text{ip_C3H7CHO2VINYL})$	Sander et al. (2019)*
J44038	TrGJC	$\text{IPRCHO} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_IPRCHO2HCO})$	Sander et al. (2019)
J44039	TrGJCN	$\text{IC4H9NO}_3 + h\nu \rightarrow \text{IPRCHO} + \text{NO}_2$	J_IC3H7NO_3	Sander et al. (2019)
J44040	TrGJC	$\text{IC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{IPRCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44041	TrGJC	$\text{PERIBUACID} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44042	TrGJCN	$\text{PIP} + h\nu \rightarrow .7 \text{IPRCO}_3 + .7 \text{NO}_2 + .3 \text{iC}_3\text{H}_7\text{O}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2019), Sander et al. (2014)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44043	TrGJC	HVMK + $h\nu$ → MGLYOX + CO + 2 OH	jx(ip_PeDIONE24)	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	HMAC + $h\nu$ → HCOCCH ₃ CO + 2 OH	jx(ip_PeDIONE24)	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	CO ₂ C ₃ CHO + $h\nu$ → CH ₃ COCH ₂ O ₂ + HO ₂ + CO	jx(ip_C2H5CHO2HCO)	Rickard and Pascoe (2009)
J44045b	TrGJC	CO ₂ C ₃ CHO + $h\nu$ → HVMK	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Sander et al. (2019)
J44046a	TrGJC	IBUTDIAL + $h\nu$ → CH ₃ CHO + CO + HO ₂ + CO ₂ + H ₂ O	jx(ip_C2H5CHO2HCO)*2.	see note*
J44046b	TrGJC	IBUTDIAL + $h\nu$ → HMAC	jx(ip_C2H5CHO2ENOL)*2.	Andrews et al. (2012), Sander et al. (2019)
J44200	TrGJTerC	IBUTALOH + $h\nu$ → CH ₃ COCH ₃ + HO ₂ + HO ₂ + CO	J_ACETOL	Rickard and Pascoe (2009)
J44201	TrGJTerC	IPRHOCO ₃ H + $h\nu$ → CH ₃ COCH ₃ + HO ₂ + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44400a	TrGJAroC	MALDIALOOH + $h\nu$ → C ₃ OH ₁₃ CO + CO + OH + HO ₂	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J44400b	TrGJAroC	MALDIALOOH + $h\nu$ → GLYOX + GLYOX + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44401	TrGJAroC	BZFUOOH + $h\nu$ → CO ₁₄ O ₃ CHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44402	TrGJAroC	HOCOC ₄ DIAL + $h\nu$ → HCOCO ₃ H + HO ₂ + CO	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44403	TrGJAroCN	NBZFUOOH + $h\nu$ → .5 CO ₁₄ O ₃ CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	MALDALCO ₃ H + $h\nu$ → HCOCO ₃ H + HO ₂ + CO + HO ₂ + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J44404b	TrGJAroC	MALDALCO ₃ H + $h\nu$ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44405	TrGJAroC	EPXDLCO ₂ H + $h\nu$ → C ₃ DIALO ₂ + CO ₂ + HO ₂	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44406	TrGJAroC	MALDIAL + $h\nu$ → .4 BZFUONE + .6 MALDIALCO ₃ + .6 HO ₂	jx(ip_NO2)*0.14	Rickard and Pascoe (2009)
J44407	TrGJAroC	MALANHYOOH + $h\nu$ → HCOCO ₃ H + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44408	TrGJAroC	EPXDLCO ₃ H + $h\nu$ → C ₃ DIALO ₂ + OH + CO ₂	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44409	TrGJAroC	CO ₂ C ₄ DIAL + $h\nu$ → CO + CO + HO ₂ + HO ₂ + CO + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
J44410	TrGJAroC	MALDALCO ₂ H + $h\nu$ → HCOCO ₂ H + HO ₂ + CO + HO ₂ + CO	jx(ip_MACR)	Rickard and Pascoe (2009)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44411	TrGJAroC	EPXC4DIAL + $h\nu$ → C3DIALO2 + CO + HO ₂	2.77*jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J44412	TrGJAroC	CO14O3CHO + $h\nu$ → HO ₂ + CO + HCOCH ₂ O ₂ + CO ₂	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44414	TrGJAroC	MECOACEOOH + $h\nu$ → CH ₃ C(O) + HCHO + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45002	TrGJC	LISOPACOOH + $h\nu$ → LISOPACO + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45003	TrGJCN	LISOPACNO3 + $h\nu$ → LISOPACO + NO ₂	0.59*J_IC3H7N03	see note*
J45004	TrGJC	ISOPBOOH + $h\nu$ → MVK + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45005	TrGJCN	ISOPBNO3 + $h\nu$ → MVK + HCHO + HO ₂ + NO ₂	2.84*J_IC3H7N03	see note*
J45006	TrGJC	ISOPDOOH + $h\nu$ → MACR + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45007	TrGJCN	ISOPDNO3 + $h\nu$ → MACR + HCHO + HO ₂ + NO ₂	J_IC3H7N03	see note*
J45008	TrGJCN	NISOPOOH + $h\nu$ → NC4CHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45009	TrGJCN	NC4CHO + $h\nu$ → LHC4ACCO3 + NO ₂	(.59*J_IC3H7N03+jx(ip_MACR)) *(jx(ip_MEKNO3)+1E-10)/(J_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)	Müller et al. (2014), Sander et al. (2019)*
J45010	TrGJCN	LNISOOH + $h\nu$ → NOA + OH + .5 HOCHCHO + .5 CO + .5 HO ₂ + .5 CO ₂	jx(ip_CH300H)	Taraborrelli et al. (2009), Sander et al. (2019)
J45011	TrGJC	LHC4ACCHO + $h\nu$ → .5 LHC4ACCO3 + .5 HO ₂ + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2	jx(ip_MACR)	Sander et al. (2019)
J45012	TrGJC	LC578OOH + $h\nu$ → .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)	Sander et al. (2019)
J45013	TrGJC	LHC4ACCO3H + $h\nu$ → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO ₂	J_HPALD	Sander et al. (2019)
J45014	TrGJCN	LC5PAN1719 + $h\nu$ → .7 LHC4ACCO3 + .7 NO ₂ + .15 MACRO2 + .15 LHMVKABO2 + .3 CO ₂ + .3 NO ₃	jx(ip_PAN)	Sander et al. (2019)
J45015	TrGJC	HCOC5 + $h\nu$ → .65 CH ₃ + .65 CO + .65 HCHO + .35 OH + .35 CH ₃ COCH ₂ O ₂ + HOCH2CO	0.5*jx(ip_MVK)	Sander et al. (2019)*
J45016	TrGJC	C59OOH + $h\nu$ → CH ₃ COCH ₂ OH + HOCH2CO + OH	J_ACETOL+jx(ip_CH300H)	Sander et al. (2019)
J45017	TrGJTerC	C511OOH + $h\nu$ → CH ₃ C(O) + HCOCH2CHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018a	TrGJTerC	CO23C4CHO + $h\nu$ → CH ₃ COCOCH ₂ O ₂ + HO ₂ + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018b	TrGJTerC	CO23C4CHO + $h\nu$ → CH ₃ C(O) + HCOCH2CO3	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45019	TrGJTerC	CO23C4CO3H + $h\nu$ → CH ₃ COCOCH ₂ O ₂ + CO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45020	TrGJTerC	C512OOH + $h\nu$ → C513O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45021	TrGJTerC	CO13C4CHO + $h\nu$ → CHOC3COO2 + CO + HO ₂	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45022	TrGJTerC	C513OOH + $h\nu$ → GLYOX + HOC ₂ H ₄ CO ₃ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45023	TrGJTerC	C513CO + $h\nu$ → HOC ₂ H ₄ CO ₃ + HO ₂ + CO + CO	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45024	TrGJTerC	$C514OOH + h\nu \rightarrow CO13C4CHO + HO_2 + OH$	$jx(ip_CH300H) + jx(ip_HOCH2CHO) * 2.$	Rickard and Pascoe (2009)
J45025	TrGJTerCN	$C514NO3 + h\nu \rightarrow CO13C4CHO + HO_2 + NO_2$	$J_IC3H7N03 + jx(ip_HOCH2CHO) * 2.$	Rickard and Pascoe (2009)
J45026a	TrGJC	$ZCODC23DBC0OH + h\nu \rightarrow OH + CO + HVMK + OH$	$J_HPALD * 0.6 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	$ZCODC23DBC0OH + h\nu \rightarrow OH + CO + CH_3C(O) + HOCH_2CHO$	$J_HPALD * 0.6 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	$ZCODC23DBC0OH + h\nu \rightarrow OH + CO + HMAc + OH$	$J_HPALD * 0.4 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	$ZCODC23DBC0OH + h\nu \rightarrow OH + CO + CO + CH_3COCH_2OH + HO_2$	$J_HPALD * 0.4 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	$LZCO3HC23DBCOD + h\nu \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO_2 + OH + CO_2$	J_HPALD	Sander et al. (2019)
J45028a	TrGJC	$C10OHC20OHC4OD + h\nu \rightarrow CH_3COCH_2O_2H + OH + 2 CO + HO_2$	$2.77 * JX(IP_HOCH2CHO)$	Sander et al. (2019)
J45028b	TrGJC	$C10OHC20OHC4OD + h\nu \rightarrow .5 CH_3COCH_2O_2H + .5 HOCHCHO + .5 CO_2H3CHO + .5 HCHO + 1.5 OH$	$2 * JX(IP_CH300H)$	Sander et al. (2019)
J45029	TrGC	$DB1OOH + h\nu \rightarrow DB1O_2 + OH$	$JX(IP_CH300H)$	Sander et al. (2019)
J45030	TrGC	$DB2OOH + h\nu \rightarrow .48 CH_3COCH_2OH + .52 HOCH_2CHO + .52 MGLYOX + .48 GLYOX + HO_2 + OH$	$JX(ip_CH300H)$	Sander et al. (2019)
J45031a	TrGJC	$C1ODC20OHC4OD + h\nu \rightarrow MGLYOX + HOCHCHO + OH$	$JX(ip_CH300H)$	Sander et al. (2019)
J45031b	TrGJC	$C1ODC20OHC4OD + h\nu \rightarrow CO_2H3CHO + CO + HO_2 + OH$	$2 * 2.77 * JX(IP_HOCH2CHO)$	Sander et al. (2019)
J45032	TrGJC	$C4MDIAL + h\nu \rightarrow .5 CH_3COCHCO + .5 HCOCCH_3CO + CO + HO_2 + OH$	$jx(ip_N02) * 0.1 * 0.5$	Sander et al. (2019)*
J45033	TrGCN	$DB1NO_3 + h\nu \rightarrow DB1O_2 + NO_2$	$J_IC3H7N03$	Sander et al. (2019)
J45034	TrGJTerC	$CHOC3COOOH + h\nu \rightarrow CHOC3COO_2 + CO_2 + OH$	$jx(ip_CH300H) + jx(ip_HOCH2CHO) + J_ACETOL$	Rickard and Pascoe (2009)
J45200a	TrGJTerC	$LMBOABOOH + h\nu \rightarrow HOCH_2CHO + CH_3COCH_3 + HO_2 + OH$	$jx(ip_CH300H) * .67$	Rickard and Pascoe (2009), Sander et al. (2019)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45200b	TrGJTerC	LMBOABOOH + $h\nu$ → IBUTALOH + HCHO + HO ₂ + OH	$jx(ip_CH300H)*.33$	Rickard and Pascoe (2009), Sander et al. (2019)
J45201	TrGJTerC	MBOACO + $h\nu$ → HCHO + HO ₂ + IPRHOCO3	J_ACETOL	Rickard and Pascoe (2009)
J45202	TrGJTerC	MBOCOCO + $h\nu$ → CO + HO ₂ + IPRHOCO3	$jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J45203a	TrGJTerCN	LNMBOABOOH + $h\nu$ → NO ₃ CH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + OH	$jx(ip_CH300H)*.65$	Rickard and Pascoe (2009), Sander et al. (2019)
J45203b	TrGJTerCN	LNMBOABOOH + $h\nu$ → IBUTALOH + HCHO + NO ₂ + OH	$jx(ip_CH300H)*.35$	Rickard and Pascoe (2009), Sander et al. (2019)
J45204	TrGJTerCN	NC4OHCO3H + $h\nu$ → IBUTALOH + CO ₂ + NO ₂ + OH	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J45400	TrGJAroC	C54CO + $h\nu$ → 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 + $h\nu$ → CH ₃ COCOCHO + HO ₂ + CO + HO ₂	$jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J45402	TrGJAroC	C5DIALOOH + $h\nu$ → MALDIAL + CO + HO ₂ + OH	$jx(ip_CH300H)+jx(ip_MACR)$	Rickard and Pascoe (2009)*
J45406	TrGJAroC	C5CO14OH + $h\nu$ → CH ₃ C(O) + HCOCO ₂ H + HO ₂ + CO	$jx(ip_MVK)$	Rickard and Pascoe (2009)
J45407	TrGJAroC	C5DICARB + $h\nu$ → .6 C5CO14O2 + .6 HO ₂ + .4 TLFUONE	$jx(ip_NO2)*0.2$	Rickard and Pascoe (2009)*
J45408	TrGJAroC	MC3ODBCO2H + $h\nu$ → CH ₃ COCO ₂ H + HO ₂ + CO + HO ₂ + CO	$jx(ip_MACR)$	Rickard and Pascoe (2009)
J45409	TrGJAroC	ACCOMMECHO + $h\nu$ → MECOACETO2 + HO ₂ + CO	$jx(ip_HOCH2CHO)$	Rickard and Pascoe (2009)
J45410	TrGJAroC	MMALNHOOH + $h\nu$ → CO2H3CO3 + CO ₂ + OH	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J45411	TrGJAroC	C5DICAROOH + $h\nu$ → MGLYOX + GLYOX + HO ₂ + OH	$jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL$	Rickard and Pascoe (2009)*
J45412	TrGJAroCN	NTLFUOOH + $h\nu$ → ACCOMECHO + NO ₂ + OH	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J45414	TrGJAroC	C5CO14OOH + $h\nu$ → .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 + $h\nu$ → ACCOMECHO + HO ₂ + OH	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J45417	TrGJAroC	ACCOMECO3H + $h\nu$ → MECOACETO2 + CO ₂ + OH	$jx(ip_CH300H)$	Rickard and Pascoe (2009)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45418	TrGJAroC	$C5DIALCO + h\nu \rightarrow MALDIALCO3 + CO + HO_2$	$jx(ip_MGLYOX) + jx(ip_MACR)$	Rickard and Pascoe (2009)
J46200	TrGJTerCN	$C614NO3 + h\nu \rightarrow CO23C4CHO + HCHO + HO_2 + NO_2$	$2.15*jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46201	TrGJTerC	$C614OOH + h\nu \rightarrow CO23C4CHO + HCHO + HO_2 + OH$	$jx(ip_CH300H) + 2.15*jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46202	TrGJTerC	$CO235C5CHO + h\nu \rightarrow CO23C4CO3 + CO + HO_2$	$jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46203	TrGJTerC	$CO235C6OOH + h\nu \rightarrow CO23C4CO3 + HCHO + OH$	$jx(ip_CH300H) + 2.15*jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46400	TrGJAroC	$PHENO OH + h\nu \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46401	TrGJAroC	$C6CO4DB + h\nu \rightarrow C4CO2DBCO3 + HO_2 + CO$	$jx(ip_MGLYOX)*2$	Rickard and Pascoe (2009)
J46402	TrGJAroC	$C5CO2DCO3H + h\nu \rightarrow CH_3C(O) + HCOCOCHO + CO_2 + OH$	$jx(ip_CH300H) + jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46403	TrGJAroCN	$NDNPHENO OH + h\nu \rightarrow NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	$BZBIPERNO3 + h\nu \rightarrow GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + NO_2$	J_IC3H7N03	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	$HOC6H4NO2 + h\nu \rightarrow HONO + CPDKETENE$	$jx(ip_HOC6H4NO2)$	Chen et al. (2011)*
J46406	TrGJAroC	$CPDKETENE + h\nu \rightarrow CO_2 + CO + 2 HO_2 + MALDIAL$	J_KETENE	see note*
J46407	TrGJAroC	$C5COOHCO3H + h\nu \rightarrow HOCOC4DIAL + HO_2 + CO + CO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46408	TrGJAroC	$BZEPOXMUC + h\nu \rightarrow .5 C5DIALO2 + 1.5 HO_2 + 1.5 CO + .5 MALDIAL$	$4.E3*jx(ip_MVK)*0.1$	Rickard and Pascoe (2009)
J46409	TrGJAroCN	$NPHEN1OOH + h\nu \rightarrow NPHEN1O + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46410	TrGJAroC	$BZEMUCCO + h\nu \rightarrow HCOCOHCOC3 + C3DIALO2$	$jx(ip_HOCH2CHO)*2 + J_ACETOL$	Rickard and Pascoe (2009)
J46411	TrGJAroC	$BZEMUCCO2H + h\nu \rightarrow C5DIALO2 + CO_2 + HO_2$	$jx(ip_MACR)$	Rickard and Pascoe (2009)
J46412	TrGJAroCN	$NNCATECOOH + h\nu \rightarrow NC4DCO2H + HCOCO2H + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46413	TrGJAroC	$C615CO2OOH + h\nu \rightarrow C5DICARB + CO + HO_2 + OH$	$jx(ip_MVK) + jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46414	TrGJAroCN	$NPHENO OH + h\nu \rightarrow MALDALCO2H + GLYOX + OH + NO_2$	$J_IC3H7N03 + jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46415	TrGJAroCN	$NCATECOOH + h\nu \rightarrow NC4DCO2H + HCOCO2H + HO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46416	TrGJAroC	$PBZQOOH + h\nu \rightarrow C5CO2OHCO3 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46417	TrGJAroC	$BZOBIPEROH + h\nu \rightarrow MALDIALCO3 + GLYOX + HO_2$	J_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	$BZBIPERO OH + h\nu \rightarrow GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	$NBZQOOH + h\nu \rightarrow C6CO4DB + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46420	TrGJAroC	CATEC1OOH + hν → CATEC1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46421	TrGJAroC	C6125CO + hν → C5CO14O2 + CO + HO ₂	jx(ip_MGLYOX)+jx(ip_MVK)	Rickard and Pascoe (2009)
J46422	TrGJAroCN	DNPHEOOH + hν → NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
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_HOC6H4NO2)	Sander et al. (2019)
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)	Wallington et al. (2018)
J47404	TrGJAroC	TLBIPEROOH + hν → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .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 C4MDIAL + .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)*

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47408b	TrGJAroCN	NCRESOOH + hν → C5CO14OH + GLYOX + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	TOL1OHNO2 + hν → HONO + MCPDKETENE	jx(ip_HOPh3Me2NO2)	see note*
J47410	TrGJAroC	TLEMUCCO2H + hν → C615CO2O2 + CO ₂ + HO ₂	jx(ip_MACR)	Rickard and Pascoe (2009)
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_HOPh3Me2NO2)	see note*
J47418	TrGJAroC	MCPDKETENE + hν → CO ₂ + CO + 2 HO ₂ + C4MDIAL	J_KETENE	see note*
J47419	TrGJAroCN	DNCRES + hν → HONO + MNCPKETENE	jx(ip_HOPh3Me2NO2)	see note*
J47420	TrGJAroCN	MNCPKETENE + 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 → C5CO2DBCO3 + 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)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J48200	TrGJTerC	$C86OOH + h\nu \rightarrow C511O2 + CH_3COCH_3 + OH$	$jx(ip_CH300H) + jx(ip_HOCH2CHO)$	Rickard and Pascoe (2009)
J48201	TrGJTerC	$C812OOH + h\nu \rightarrow C813O2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J48202	TrGJTerC	$C813OOH + h\nu \rightarrow CH_3COCH_3 + C512O2 + OH$	$jx(ip_CH300H) + jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J48203	TrGJTerC	$C721CHO + h\nu \rightarrow C721O2 + CO + HO_2$	$jx(ip_HOCH2CHO)$	Rickard and Pascoe (2009)
J48204	TrGJTerC	$C721CO3H + h\nu \rightarrow C721O2 + CO_2 + OH$	$jx(ip_CH300H)$	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), Sander et al. (2019)
J49203b	TrGJTerC	$NORPINAL + h\nu \rightarrow NORPINENOL$	$jx(ip_PINAL2ENOL)$	Sander et al. (2019), 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	$PINAL + h\nu \rightarrow PINEOL$	$jx(ip_PINAL2ENOL)$	Sander et al. (2019), Andrews et al. (2012)*
J40204	TrGJTerC	$PERPINONIC + h\nu \rightarrow C96O2 + CO_2 + OH$	$jx(ip_CH300H) + J_ACETOL$	Rickard and Pascoe (2009)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J40205	TrGJTerC	PINALOOH + $h\nu$ → C106O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40206	TrGJTerCN	PINALNO3 + $h\nu$ → C106O2 + NO ₂	J_IC3H7N03+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40207	TrGJTerC	C106OOH + $h\nu$ → C716O2 + CH ₃ COCH ₃ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40208	TrGJTerCN	C106NO3 + $h\nu$ → C716O2 + CH ₃ COCH ₃ + NO ₂	J_IC3H7N03+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40209	TrGJTerC	C109OOH + $h\nu$ → C89CO3 + HCHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40210	TrGJTerC	C109CO + $h\nu$ → C89CO3 + CO + HO ₂	jx(ip_MGLY0X)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40211	TrGJTerCN	LNAPINABOOH + $h\nu$ → PINAL + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40212	TrGJTerC	BPINAOOH + $h\nu$ → NOPINONE + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40213	TrGJTerCN	LNBPINABOOH + $h\nu$ → NOPINONE + HCHO + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40214	TrGJTerCN	ROO6R1NO3 + $h\nu$ → ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	2.84*J_IC3H7N03+jx(ip_CH300H)	Sander et al. (2019)
J40215	TrGJTerCN	RO6R1NO3 + $h\nu$ → 9 LCARBON + HCHO + HO ₂ + NO ₂	2.84*J_IC3H7N03	Sander et al. (2019)
J6000	StTrGJCl	Cl ₂ + $h\nu$ → Cl + Cl	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	Cl ₂ O ₂ + $h\nu$ → 2 Cl	jx(ip_Cl202)	Sander et al. (2014)
J6101	StTrGJCl	OCIO + $h\nu$ → ClO + O(³ P)	jx(ip_OC10)	Sander et al. (2014)
J6200	StGJCl	HCl + $h\nu$ → Cl + H	jx(ip_HCl)	Sander et al. (2014)
J6201	StTrGJCl	HOCl + $h\nu$ → OH + Cl	jx(ip_HOCl)	Sander et al. (2014)
J6300	TrGJClN	ClNO ₂ + $h\nu$ → Cl + NO ₂	jx(ip_Cl1N02)	Sander et al. (2014)
J6301a	StTrGJClN	ClNO ₃ + $h\nu$ → Cl + NO ₃	jx(ip_Cl1N03)	Sander et al. (2014)
J6301b	StTrGJClN	ClNO ₃ + $h\nu$ → ClO + NO ₂	jx(ip_Cl1ON02)	Sander et al. (2014)
J6400	StGJCl	CH ₃ Cl + $h\nu$ → Cl + CH ₃	jx(ip_CH3Cl)	Sander et al. (2014)
J6401	StGJCl	CCl ₄ + $h\nu$ → LCARBON + 4 Cl	jx(ip_CC14)	Sander et al. (2014)
J6402	StGJCCl	CH ₃ CCl ₃ + $h\nu$ → 2 LCARBON + 3 Cl	jx(ip_CH3CC13)	Sander et al. (2014)
J6500	StGJClF	CFCl ₃ + $h\nu$ → LCARBON + LFLUORINE + Cl + 2 LCHLORINE	jx(ip_CFC13)	Sander et al. (2014)*
J6501	StGJClF	CF ₂ Cl ₂ + $h\nu$ → LCARBON + 2 LFLUORINE + Cl + LCHLORINE	jx(ip_CF2Cl2)	Sander et al. (2014)*
J7000	StTrGJBr	Br ₂ + $h\nu$ → Br + Br	jx(ip_Br2)	Sander et al. (2014)
J7100	StTrGJBr	BrO + $h\nu$ → Br + O(³ P)	jx(ip_Br0)	Sander et al. (2014)
J7200	StTrGJBr	HOBr + $h\nu$ → Br + OH	jx(ip_HOBr)	Sander et al. (2014)
J7300	TrGJBrN	BrNO ₂ + $h\nu$ → Br + NO ₂	jx(ip_BrN02)	Sander et al. (2014)
J7301	StTrGJBrN	BrNO ₃ + $h\nu$ → .85 Br + .85 NO ₃ + .15 BrO + .15 NO ₂	jx(ip_BrN03)	Sander et al. (2014)*
J7400	StGJBr	CH ₃ Br + $h\nu$ → Br + CH ₃	jx(ip_CH3Br)	Sander et al. (2014)
J7401	TrGJBr	CH ₂ Br ₂ + $h\nu$ → LCARBON + 2 Br	jx(ip_CH2Br2)	Sander et al. (2014)
J7402	TrGJBr	CHBr ₃ + $h\nu$ → LCARBON + 3 Br	jx(ip_CHBr3)	Sander et al. (2014)
J7500	StGJBrF	CF ₃ Br + $h\nu$ → LCARBON + 3 LFLUORINE + Br	jx(ip_CF3Br)	Sander et al. (2014)

Table S2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGJBrCl	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_BrCl})$	Sander et al. (2014)
J7601	StGJBrClF	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + 2 \text{LFLUORINE} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CF2ClBr})$	Sander et al. (2014)
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CH2ClBr})$	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{LCARBON} + \text{Br} + 2 \text{Cl}$	$\text{jx}(\text{ip_CHCl2Br})$	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CHClBr2})$	Sander et al. (2014)
J9000	TrStGJS	$\text{OCS} + h\nu \rightarrow \text{CO} + \text{S}$	$\text{JX}(\text{ip_OCS})$	Brühl et al. (2012)
J9001	TrStGJS	$\text{SO}_2 + h\nu \rightarrow \text{SO} + \text{O}(^3\text{P})$	$60.*\text{JX}(\text{ip_OCS})$	Brühl et al. (2012)
J9002	TrStGJS	$\text{SO}_3 + h\nu \rightarrow \text{SO}_2 + \text{O}(^3\text{P})$	$\text{JX}(\text{ip_SO3})$	Brühl et al. (2012)
J9003	TrStGJS	$\text{H}_2\text{SO}_4 + h\nu \rightarrow \text{SO}_3 + \text{H}_2\text{O}$	$\text{JX}(\text{ip_H2SO4})$	Brühl et al. (2012)
PH (aqueous)				

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:

$\text{J}(11) \rightarrow \text{jx}(\text{ip_COH2})$
 $\text{J}(12) \rightarrow \text{jx}(\text{ip_CHOH})$
 $\text{J}(15) \rightarrow \text{jx}(\text{ip_HOCH2CHO})$
 $\text{J}(18) \rightarrow \text{jx}(\text{ip_MACR})$
 $\text{J}(22) \rightarrow \text{jx}(\text{ip_ACETOL})$
 $\text{J}(23)+\text{J}(24) \rightarrow \text{jx}(\text{ip_MVK})$
 $\text{J}(31)+\text{J}(32)+\text{J}(33) \rightarrow \text{jx}(\text{ip_GLYOX})$
 $\text{J}(34) \rightarrow \text{jx}(\text{ip_MGLYOX})$
 $\text{J}(41) \rightarrow \text{jx}(\text{ip_CH3OOH})$
 $\text{J}(53) \rightarrow \text{J}(\text{isopropyl nitrate})$
 $\text{J}(54) \rightarrow \text{J}(\text{isopropyl nitrate})$
 $\text{J}(55) \rightarrow \text{J}(\text{isopropyl nitrate})$
 $\text{J}(56)+\text{J}(57) \rightarrow \text{jx}(\text{ip_NOA})$

Specific notes

J41003: CH_3 - and CH_2 -channels are considered only and with their branching ratios being 0.42 and 0.48, respectively (Gans et al., 2011). CH -production is neglected. CH_2 is assumed to react only with O_2 yielding $1.44 \text{H}_2 + .18 \text{HCHO} + .18 \text{O}(^3\text{P}) + .33 \text{OH} + .33 \text{HO}_2 + .44 \text{CO}_2 + .38 \text{CO} + .05 \text{H}_2\text{O}$ as assumed in the WACCM model by J. Orlando (Doug Kinnison, pers. comm. with D. Taraborrelli).

J41006: product distribution as for HNO_4

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

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

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

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

J42007: It is assumed that $\text{J}(\text{PHAN})$ is the same as $\text{J}(\text{PAN})$.

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

J42020: It is assumed that $\text{J}(\text{NO}_3\text{CH}_2\text{CHO})$ is the same as $\text{J}(\text{PAN})$.

J42021: In analogy to what is assumed for $\text{CH}_3\text{O}_2\text{NO}_2$ photolysis as in (Sander et al., 2014).

J43002: Following von Kuhlmann et al. (2003), we use $\text{J}(\text{CH}_3\text{COCH}_2\text{OH}) = 0.11*\text{jx}(\text{ip_CHOH})$. 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 $\text{J}(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7*\text{jx}(\text{ip_PAN})$.

J43018: One third of the acetaldehyde channel is considered to be CH_2CHOH according to Hjorth (2002) EUPHORE Report.

J43024: Assuming $\text{J}(\text{C}_3\text{H}_7\text{ONO}_2) = 0.59 \times \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

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

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

J43400: $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

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 CH₃COCH which upon reaction with O₂ 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*J_IC3H7NO3 like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to Müller et al. (2014).

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

J44043: The resulting vinyl peroxy radical is assumed to mostly form with HO₂ a labile hydroperoxide (see ketene formation). The products are further simplified.

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

J44046a: Simplified oxidation.

J44400b: KDEC MALDIALO → GLYOX + GLYOX + HO₂

J44401: KDEC BZFUO → CO₁₄O₃CHO + HO₂

J44403: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂

J44404b: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO

J44407: KDEC MALANHYO → HCOCO₂HCO₃

J44414: KDEC MECOACETO → CH₃CO₃ + HCHO

J45003: It is assumed that J(LISOPACNO₃) = 0.59 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that J(ISOPBNO₃) = 2.84 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that J(ISOPDNO₃) is the same as J(iC₃H₇ONO₂).

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

J45015: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that J(HCOC₅) is half as large as J(MVK). With exception of HOCH₂CO the products of MACO₂ decomposition without CO₂.

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

J45402: KDEC C5DIALO → MALDIAL + CO + HO₂

J45407: KDEC TLFUONE → .6 C5CO₁₄O₂ + .6 HO₂ + .4 TLFUONE

J45410: KDEC MMALANHYO → CO₂H₃CO₃

J45411: KDEC C5DICARBO → MGLYOX + GLYOX + HO₂

J45412: KDEC NTLFUO → ACCOMECHO + NO₂

J45414: KDEC C5CO₁₄CO₂ → .83 MALANHY + .83 CH₃ + .17 MGLYOX + .17 HO₂ + .17 CO + .17 CO₂

J45415: KDEC TLFUO → ACCOMECHO + HO₂

J46400: KDEC PHENO → .71 MALDALCO₂H + .71 GLYOX + .29 PBZQONE + HO₂

J46403: KDEC NDNPHENO → NC₄D_{CO}₂H + HNO₃ + CO + CO + NO₂

J46404: KDEC BZBIPERO → GLYOX + HO₂ + .5 BZFUONE + .5 BZFUONE

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO → NC₄D_{CO}₂H + HCOCO₂H + NO₂

J46415: KDEC NCATECO → NC₄D_{CO}₂H + HCOCO₂H + HO₂

J46416: KDEC PBZQO → C₅CO₂OHCO₃

J46418: KDEC BZBIPERO → GLYOX + HO₂ + .5 BZFUONE + .5 BZFUONE

J46419: KDEC NBZQO → C₆CO₄DB + NO₂

J46422: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

J46425: KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

J46429: new channel

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

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

J47404: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

J47405: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

J47407: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

J47408a: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

J47408b: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

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

J47412: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

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

J47418: new channel

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

J47420: new channel

J47422: KDEC NPTLQO \rightarrow C7CO4DB + NO2

J47423: KDEC PTLQO \rightarrow C6CO2OHCO3

J47425: KDEC MNNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

J47426: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

J47428: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

J47429: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

J48400: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

J40203b: Substituted vinyl alcohol in analogy to CH₃CHO photolysis.

J6500: Only 1 Cl atom is produced (Felder and Demuth, 1993).

J6501: Only 1 Cl atom is produced in analogy to CFC1₃.

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

Table S3: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
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General notes

The forward (k_{exf}) and backward (k_{exb}) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry’s law constants from `chemprop` (see `chemprop.pdf`).

For uptake of X ($X = \text{N}_2\text{O}_5, \text{ClNO}_3, \text{or BrNO}_3$) and

subsequent reaction with H_2O , Cl^- , and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

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

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 reactions. 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 N_2O_5 . Here, they are also used for ClNO_3 and BrNO_3 .

Table S4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2 \text{HNO}_3$	<code>khet_St(ihs_N2O5_H2O)</code>	see general notes*
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^-(\text{cs}) + 2 \text{H}^+(\text{cs})$	<code>khet_Tr(iht_N2O5)</code>	see general notes*
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see general notes*
HET420	StHetClN	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see general notes*
HET421	StHetClN	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H2O)</code>	see general notes*
HET422	StHetClN	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N2O5_HCl)</code>	see general notes*
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see general notes*
HET520	StHetBrN	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H2O)</code>	see general notes*
HET540	StHetBrClN	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see general notes*
HET541	StHetBrClN	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see general notes*
HET542	StHetBrCl	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see general notes*
HET543	StHetBrCl	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HCl)</code>	see general notes*

General notes

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

Table S5: Acid-base and other equilibria

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

Table S6: Aqueous phase reactions

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

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