Table 1: Gas phase reactions

reaction	rate coefficient	reference		
Aro001	TrGC	C5DICARBO2 + HO_2 → C5DICAROOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro002	TrGC	C5DICARBO2 + HO_2 → MGLYOX + GLYOX + HO_2 + OH	KRO2HO2*0.706*(rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro003	TrGCN	C5DICARBO2 + NO → MGLYOX + GLYOX + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro004	TrGCN	C5DICARBO2 + NO_3 → MGLYOX + GLYOX + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro005	TrGC	C5DICARBO2 → MGLYOX + GLYOX + HO_2	KRO2sHORO2*RO2	Rickard and Pascoe (2009)*
Aro006	TrGC	MCOCOMOOOH + OH → MCOCOMOXO2	2.00E-11	Rickard and Pascoe (2009)
Aro007	TrGC	C33CO + OH → CO + CO + CO + HO_2	5.77E-11	Rickard and Pascoe (2009)
Aro008	TrGC	C3DIALOOH + OH → C33CO + OH	1.44E-10	Rickard and Pascoe (2009)
Aro009	TrGC	C3DIALO2 + HO_2 → C3DIALOOH	KRO2HO2*0.520*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro010	TrGC	C3DIALO2 + HO_2 → GLYOX + CO + HO_2 + OH	KRO2HO2*0.520*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro011	TrGCN	C3DIALO2 + NO → GLYOX + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro012	TrGCN	C3DIALO2 + NO_3 → GLYOX + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro013	TrGC	C3DIALO2 → GLYOX + CO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro014	TrGC	HCOCOHCO3 + HO_2 → GLYOX + HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro015	TrGC	HCOCOHCO3 + HO_2 → HCOCOHCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro016	TrGCN	HCOCOHCO3 + NO → GLYOX + HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro017	TrGCN	HCOCOHCO3 + NO_2 → HCOCOHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
Aro018	TrGCN	HCOCOHCO3 + NO_3 → GLYOX + HO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro019	TrGC	HCOCOHCO3 → GLYOX + HO_2	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro020	TrGC	METACETHO + OH → $CH_3C(O)OO$	9.82E-11	Rickard and Pascoe (2009)
Aro021	TrGC	C5DIALCO + OH → MALDIALCO3 + CO	4.90E-11	Rickard and Pascoe (2009)
Aro022	TrGCN	HCOCOHPAN + OH → GLYOX + CO + NO_2	6.97E-11	Rickard and Pascoe (2009)
Aro023	TrGCN	HCOCOHPAN → HCOCOHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
Aro024	TrGC	C32OH13CO + OH → HCOCOHCO3	1.36E-10	Rickard and Pascoe (2009)
Aro025	TrGC	HCOCOHCO3H + OH → HCOCOHCO3	7.33E-11	Rickard and Pascoe (2009)
Aro026	TrGC	MALANHY + OH → MALANHYO2	1.4E-12	Rickard and Pascoe (2009)
Aro027	TrGC	MALDIALOOH + OH → HOCOC4DIAL + OH	1.22E-10	Rickard and Pascoe (2009)
Aro028	TrGC	MALDIALOOH + OH → MALDIALO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro029	TrGCN	NC4DCO2H + OH → MALANHY + NO_2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)*
Aro030	TrGC	CO14O3CO2H + OH → HCOCH2O2	2.19E-11	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro031	TrGC	BZFUOOH + OH → BZFUO2	3.68E-11	Rickard and Pascoe (2009)
Aro032	TrGC	HOCOC4DIAL + OH → CO2C4DIAL + HO_2	3.67E-11	Rickard and Pascoe (2009)
Aro033	TrGC	MALDIALCO3 + HO_2 → MALDALCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro034	TrGC	MALDIALCO3 + HO_2 → MALDALCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro035	TrGC	MALDIALCO3 + HO_2 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro036	TrGCN	MALDIALCO3 + NO → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + NO_2	KAPNO	Rickard and Pascoe (2009)*
Aro037	TrGCN	MALDIALCO3 + NO_2 → MALDIALPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
Aro038	TrGCN	MALDIALCO3 + NO_3 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*
Aro039	TrGC	MALDIALCO3 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro040	TrGCN	BZFUONE + NO_3 → NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
Aro041	TrGC	BZFUONE + O_3 → .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H_2O_2 + .5 CO + .5 HCOCH2O2 + .5 OH	2.20E-19	Rickard and Pascoe (2009)*
Aro042	TrGC	BZFUONE + OH → BZFUO2	4.45E-11	Rickard and Pascoe (2009)
Aro043	TrGCN	NBZFUOOH + OH → NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
Aro044	TrGC	MALDALCO3H + OH → MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
Aro045	TrGC	EPXDLCO2H + OH → C3DIALO2	2.31E-11	Rickard and Pascoe (2009)
Aro046	TrGC	EPXDLCO3 + HO_2 → C3DIALO2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro047	TrGC	EPXDLCO3 + HO_2 → EPXDLCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro048	TrGC	EPXDLCO3 + HO_2 → EPXDLCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro049	TrGCN	EPXDLCO3 + NO → C3DIALO2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro050	TrGCN	EPXDLCO3 + NO_2 → EPXDLPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
Aro051	TrGCN	EPXDLCO3 + NO_3 → C3DIALO2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro052	TrGC	EPXDLCO3 → C3DIALO2	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro053	TrGC	MALNHYOHCO + OH → CO + CO + CO + HO_2	5.68E-12	Rickard and Pascoe (2009)
Aro054	TrGCN	MALDIAL + NO_3 → MALDIALCO3 + HNO_3	2*KNO3AL*2.0	Rickard and Pascoe (2009)
Aro055	TrGC	MALDIAL + O_3 → 1.0675 GLYOX + .125 HCHO + .1125 $HCOCO_2H$ + .0675 H_2O_2 + 0.82 HO_2 + .57 OH + 1.265 CO	2.00E-18	Rickard and Pascoe (2009)*
Aro056	TrGC	MALDIAL + OH → .83 MALDIALCO3 + .17 MALDIALO2	5.20E-11	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro057	TrGC	MALANHYOOH + OH → MALNHYOHCO + OH	4.66E-11	Rickard and Pascoe (2009)
Aro058	TrGCN	MALDIALPAN + OH → GLYOX + CO + CO + NO_2	3.70E-11	Rickard and Pascoe (2009)
Aro059	TrGCN	MALDIALPAN → MALDIALCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
Aro060	TrGC	MALANHYO2 + HO_2 → MALANHYOOH	KRO2HO2*0.625*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro061	TrGC	MALANHYO2 + HO_2 → HCOCOHCO3 + OH	KRO2HO2*0.625*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro062	TrGCN	MALANHYO2 + NO → HCOCOHCO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro063	TrGCN	MALANHYO2 + NO_3 → HCOCOHCO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro064	TrGC	MALANHYO2 → HCOCOHCO3	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro065	TrGC	EPXDLCO3H + OH → EPXDLCO3	2.62E-11	Rickard and Pascoe (2009)
Aro066	TrGC	CO2C4DIAL + OH → CO + CO + CO + CO + HO_2	2.45E-11	Rickard and Pascoe (2009)
Aro067	TrGC	NBZFUO2 + HO_2 → NBZFUOOH	KRO2HO2*0.625*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro068	TrGC	NBZFUO2 + HO_2 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + OH	KRO2HO2*0.625*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro069	TrGCN	NBZFUO2 + NO → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro070	TrGCN	NBZFUO2 + NO_3 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro071	TrGCN	NBZFUO2 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro072	TrGC	MALDALCO2H + OH → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO	3.70E-11	Rickard and Pascoe (2009)*
Aro073	TrGCN	EPXC4DIAL + NO_3 → EPXDLCO3 + HNO_3	2*KNO3AL*4.0	Rickard and Pascoe (2009)
Aro074	TrGC	EPXC4DIAL + OH → EPXDLCO3	4.32E-11	Rickard and Pascoe (2009)
Aro075	TrGC	MECOACETO2 + HO_2 → MECOACEOOH	KRO2HO2*0.625*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro076	TrGC	MECOACETO2 + HO_2 → $CH_3C(O)OO$ + HCHO + OH	KRO2HO2*0.625*(rcoch2o2_oh)	Rickard and Pascoe (2009)*
Aro077	TrGCN	MECOACETO2 + NO → $CH_3C(O)OO$ + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro078	TrGCN	MECOACETO2 + NO_3 → $CH_3C(O)OO$ + HCHO + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro079	TrGC	MECOACETO2 → $CH_3C(O)OO$ + HCHO	KRO2pORO2*RO2	Rickard and Pascoe (2009)*
Aro080	TrGCN	CO14O3CHO + NO_3 → CO + HCOCH2O2 + HNO_3	KNO3AL*8.0	Rickard and Pascoe (2009)
Aro081	TrGC	CO14O3CHO + OH → CO + HCOCH2O2	3.44E-11	Rickard and Pascoe (2009)
Aro082	TrGCN	NBZFUONE + OH → BZFUCO + NO_2	1.16E-12	Rickard and Pascoe (2009)
Aro083	TrGC	BZFUO2 + HO_2 → BZFUOOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro084	TrGC	BZFUO2 + HO_2 → CO14O3CHO + HO_2 + OH	KRO2HO2*0.706*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro085	TrGCN	BZFUO2 + NO → CO14O3CHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro086	TrGCN	BZFUO2 + NO_3 → CO14O3CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro087	TrGC	BZFUO2 → CO14O3CHO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro088	TrGC	BZFUCO + OH → CO14O3CHO + HO_2	1.78E-11	Rickard and Pascoe (2009)
Aro089	TrGCN	C23O3CHO + NO_3 → CO + $CH_3C(O)OO$ + HNO_3	KNO3AL*4.0	Rickard and Pascoe (2009)
Aro090	TrGC	C23O3CHO + OH → CO + $CH_3C(O)OO$	1.27E-11	Rickard and Pascoe (2009)
Aro091	TrGC	MALDIALO2 + HO_2 → MALDIALOOH	KRO2HO2*0.625*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro092	TrGC	MALDIALO2 + HO_2 → GLYOX + GLYOX + HO_2 + OH	KRO2HO2*0.625*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro093	TrGCN	MALDIALO2 + NO → GLYOX + GLYOX + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro094	TrGCN	MALDIALO2 + NO_3 → GLYOX + GLYOX + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro095	TrGC	MALDIALO2 → GLYOX + GLYOX + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro096	TrGCN	NC4MDCO2HN + OH → MMALANHY + NO_2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)*
Aro097	TrGCN	C54CO + NO_3 → CO + CO + CO + $CH_3C(O)OO$ + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
Aro098	TrGC	C54CO + OH → CO + CO + CO + $CH_3C(O)OO$	1.72E-11	Rickard and Pascoe (2009)
Aro099	TrGCN	NTLFUO2 + HO_2 → NTLFUOOH	KRO2HO2*0.706*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro100	TrGC	NTLFUO2 + HO_2 → ACCOMECHO + NO_2 + OH	KRO2HO2*0.706*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro101	TrGCN	NTLFUO2 + NO → ACCOMECHO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro102	TrGCN	NTLFUO2 + NO_3 → ACCOMECHO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro103	TrGCN	NTLFUO2 → ACCOMECHO + NO_2	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro104	TrGC	C5134CO2OH + OH → C54CO + HO_2	7.48E-11	Rickard and Pascoe (2009)
Aro105	TrGC	MC3CODBCO3 + HO_2 → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro106	TrGC	MC3CODBCO3 + HO_2 → MC3ODBCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro107	TrGC	MC3CODBCO3 + HO_2 → MC3ODBCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro108	TrGCN	MC3CODBCO3 + NO → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
Aro109	TrGCN	MC3CODBCO3 + NO_2 → MC3CODBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro110	TrGCN	MC3CODBCO3 + NO_3 → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro111	TrGCN	MC3CODBCO3 → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2	1.00E-11*RO2*0.90	Rickard and Pascoe (2009)*
Aro112	TrGCN	MC3CODBCO3 → MC3ODBCO2H	1.00E-11*RO2*0.1	Rickard and Pascoe (2009)*
Aro113	TrGCN	C5COO2NO2 + OH → MGLYOX + CO + CO + NO_2	5.43E-11	Rickard and Pascoe (2009)
Aro114	TrGCN	C5COO2NO2 → C5CO14O2 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro115	TrGC	C5DIALOOH + OH → C5DIALCO + OH	7.52E-11	Rickard and Pascoe (2009)
Aro116	TrGC	C4CO2DBCO3 + HO_2 → C4CO2DCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro117	TrGC	C4CO2DBCO3 + HO_2 → HO_2 + CO + C33CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro118	TrGCN	C4CO2DBCO3 + NO → HO_2 + CO + C33CO + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro119	TrGCN	C4CO2DBCO3 + NO_2 → C4CO2DBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro120	TrGCN	C4CO2DBCO3 + NO_3 → HO_2 + CO + C33CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro121	TrGC	C4CO2DBCO3 → HO_2 + CO + C33CO	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro122	TrGC	MMALANHY + OH → MMALANHYO2	1.50E-12	Rickard and Pascoe (2009)
Aro123	TrGC	PXYFUO2 + HO_2 → PXYFUOOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro124	TrGC	PXYFUO2 + HO_2 → C23O3CCHO + HO_2 + OH	KRO2HO2*0.706*rcoch2o2_oh+rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro125	TrGCN	PXYFUO2 + NO → C23O3CCHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro126	TrGCN	PXYFUO2 + NO_3 → C23O3CCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro127	TrGC	PXYFUO2 → C23O3CCHO + HO_2	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro128	TrGC	MMALANHYO2 + HO_2 → MMALNHYOOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro129	TrGC	MMALANHYO2 + HO_2 → CO2H3CO3 + OH	KRO2HO2*0.706*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro130	TrGCN	MMALANHYO2 + NO → CO2H3CO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro131	TrGCN	MMALANHYO2 + NO_3 → CO2H3CO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro132	TrGC	MMALANHYO2 → CO2H3CO3	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro133	TrGCN	NPXYFUOOH + OH → NPXYFUO2	5.16E-12	Rickard and Pascoe (2009)
Aro134	TrGCN	C23O3CCHO + NO_3 → C23O3CCO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
Aro135	TrGC	C23O3CCHO + OH → C23O3CCO3	2.15E-11	Rickard and Pascoe (2009)
Aro136	TrGCN	C4CO2DBPAN + OH → C33CO + CO + NO_2	2.74E-11	Rickard and Pascoe (2009)
Aro137	TrGCN	C4CO2DBPAN → C4CO2DBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro138	TrGC	C5CO14O2 + HO_2 → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro139	TrGC	C5CO14O2 + HO_2 → C5CO14OH + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro140	TrGC	C5CO14O2 + HO_2 → C5CO14OOH	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro141	TrGCN	C5CO14O2 + NO → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO + NO_2	KAPNO	Rickard and Pascoe (2009)*
Aro142	TrGCN	C5CO14O2 + NO_2 → C5COO2NO2	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro143	TrGCN	C5CO14O2 + NO_3 → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*
Aro144	TrGC	C5CO14O2 → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro145	TrGC	PXYFUOOH + OH → PXYFUO2	2.78E-11	Rickard and Pascoe (2009)
Aro146	TrGCN	MC3CODBPAN + OH → GLYOX + HCHO + CO + NO_2	4.37E-11	Rickard and Pascoe (2009)
Aro147	TrGCN	MC3CODBPAN → MC3CODBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro148	TrGC	C5CO14OH + OH → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO	5.44E-11	Rickard and Pascoe (2009)*
Aro149	TrGC	NPXYFUO2 + HO_2 → NPXYFUOOH	KRO2HO2*0.706*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro150	TrGCN	NPXYFUO2 + HO_2 → C23O3CCHO + NO_2 + OH	KRO2HO2*0.706*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro151	TrGCN	NPXYFUO2 + NO → C23O3CCHO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro152	TrGCN	NPXYFUO2 + NO_3 → C23O3CCHO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro153	TrGCN	NPXYFUO2 → C23O3CCHO + NO_2	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro154	TrGCN	C5DICARB + NO_3 → C5CO14O2 + HNO_3	KNO3AL*2.75	Rickard and Pascoe (2009)
Aro155	TrGC	C5DICARB + O_3 → .5338 GLYOX + .063 CH_3CHO + .348 $CH_3C(O)OO$ + .918 CO + .57 OH + .473 HO_2 + .0563 CH3COCO2H + .5338 MGLYOX +.676 H_2O_2 + .063 HCHO + .0563 $HCOCO_2H$	2.00E-18	Rickard and Pascoe (2009)
Aro156	TrGC	C5DICARB + OH → .48 C5CO14O2 + .52 C5DICARBO2	6.2E-11	Rickard and Pascoe (2009)
Aro157	TrGC	MC3ODBCO2H + OH → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2	4.38E-11	Rickard and Pascoe (2009)*
Aro158	TrGC	C23O3CCO2H + OH → MCOCOMOXO2	8.76E-13	Rickard and Pascoe (2009)
Aro159	TrGC	C23O3CCO3 + HO_2 → C23O3CCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro160	TrGC	C23O3CCO3 + HO_2 → C23O3CCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro161	TrGC	C23O3CCO3 + HO_2 → MCOCOMOXO2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro162	TrGCN	C23O3CCO3 + NO → MCOCOMOXO2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro163	TrGCN	C23O3CCO3 + NO_2 → C23O3CPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro164	TrGCN	C23O3CCO3 + NO_3 → MCOCOMOXO2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro165	TrGC	C23O3CCO3 → MCOCOMOXO2	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro166	TrGCN	TLFUONE + NO_3 → NTLFUO2	1.00E-12	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro167	TrGC	TLFUONE + O_3 → .5 CO + .5 OH + .5 MECOACETO2 + .3125 C24O3CCO2H + .1875 ACCOMECHO + .1875 H_2O_2	8.00E-19	Rickard and Pascoe (2009)*
Aro168	TrGC	TLFUONE + OH → TLFUO2	6.90E-11	Rickard and Pascoe (2009)
Aro169	TrGC	ACCOMECO3 + HO_2 → ACCOMECO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro170	TrGC	ACCOMECO3 + HO_2 → MECOACETO2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro171	TrGCN	ACCOMECO3 + NO → MECOACETO2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro172	TrGCN	ACCOMECO3 + NO_2 → ACCOMEPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro173	TrGCN	ACCOMECO3 + NO_3 → MECOACETO2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro174	TrGC	ACCOMECO3 → MECOACETO2	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro175	TrGC	C4CO2DCO3H + OH → C4CO2DBCO3	3.06E-11	Rickard and Pascoe (2009)
Aro176	TrGCN	EPXDLPAN + OH → C33CO + CO + NO_2	2.29E-11	Rickard and Pascoe (2009)
Aro177	TrGCN	EPXDLPAN → EPXDLCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro178	TrGC	C4M2ALOHO2 + HO_2 → C4MALOHOOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro179	TrGC	C4M2ALOHO2 + HO_2 → GLYOX + MGLYOX + HO_2 + OH	KRO2HO2*0.706*rcoch2o2_oh+rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro180	TrGCN	C4M2ALOHO2 + NO → GLYOX + MGLYOX + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro181	TrGCN	C4M2ALOHO2 + NO_3 → GLYOX + MGLYOX + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro182	TrGC	C4M2ALOHO2 → GLYOX + MGLYOX + HO_2	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro183	TrGCN	ACCOMECHO + NO_3 → ACCOMECO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
Aro184	TrGC	ACCOMECHO + OH → ACCOMECO3	7.09E-11	Rickard and Pascoe (2009)
Aro185	TrGC	MMALNHYOOH + OH → MMALANHYO2	1.69E-11	Rickard and Pascoe (2009)
Aro186	TrGC	C5DICAROOH + OH → C5134CO2OH + OH	1.21E-10	Rickard and Pascoe (2009)
Aro187	TrGC	C5DICAROOH + OH → C5DICARBO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro188	TrGC	C24O3CCO2H + OH → MECOACETO2	8.76E-13	Rickard and Pascoe (2009)
Aro189	TrGCN	NTLFUOOH + OH → NTLFUO2	4.44E-12	Rickard and Pascoe (2009)
Aro190	TrGC	MECOACEOOH + OH → MECOACETO2	3.59E-12	Rickard and Pascoe (2009)
Aro191	TrGCN	ACCOMEPAN + OH → METACETHO + CO + CO + NO_2	1.00E-14	Rickard and Pascoe (2009)
Aro192	TrGCN	ACCOMEPAN → ACCOMECO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro193	TrGC	C4MALOHOOH + OH → GLYOX + MGLYOX + HO_2	4.58E-11	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro194	TrGC	C3MCODBCO3 + HO_2 → .35 MGLYOX + .35 HO_2 + .35 CO + .65 MMALANHY + .65 HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro195	TrGC	C3MCODBCO3 + HO_2 → C4CODBCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro196	TrGCN	C3MCODBCO3 + NO → .35 MGLYOX + .35 HO_2 + .35 CO + .65 MMALANHY + .65 HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
Aro197	TrGCN	C3MCODBCO3 + NO_2 → C3MCODBPANN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro198	TrGCN	C3MCODBCO3 + NO_3 → NO_2 + .35 MGLYOX + .35 HO_2 + .35 CO + .65 MMALANHY + .65 HO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*
Aro199	TrGC	C3MCODBCO3 → .35 MGLYOX + .35 HO_2 + .35 CO + .65 MMALANHY + .65 HO_2	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro200	TrGCN	PXYFUONE + NO_3 → NPXYFUO2	1.00E-12	Rickard and Pascoe (2009)
Aro201	TrGC	PXYFUONE + O_3 → OH + CO + MCOCOMOXO2	8.00E-19	Rickard and Pascoe (2009)
Aro202	TrGC	PXYFUONE + OH → PXYFUO2	2.42E-11	Rickard and Pascoe (2009)
Aro203	TrGC	TLFUO2 + HO_2 → TLFUOOH	KRO2HO2*0.706*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro204	TrGC	TLFUO2 + HO_2 → ACCOMECHO + HO_2 + OH	KRO2HO2*0.706*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro205	TrGCN	TLFUO2 + NO → ACCOMECHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro206	TrGCN	TLFUO2 + NO_3 → ACCOMECHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro207	TrGC	TLFUO2 → ACCOMECHO + HO_2	KRO2tORO2*RO2	Rickard and Pascoe (2009)*
Aro208	TrGC	C5CO14OOH + OH → C5CO14O2	3.59E-12	Rickard and Pascoe (2009)
Aro209	TrGCN	C23O3CPAN + OH → CO + C23O3CHO + NO_2	7.36E-13	Rickard and Pascoe (2009)
Aro210	TrGCN	C23O3CPAN → C23O3CCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro211	TrGC	C4CODBCO3H + OH → C3MCODBCO3	4.73E-11	Rickard and Pascoe (2009)
Aro212	TrGC	TLFUOOH + OH → TLFUO2	2.53E-11	Rickard and Pascoe (2009)
Aro213	TrGC	C23O3CCO3H + OH → C23O3CCO3	4.34E-12	Rickard and Pascoe (2009)
Aro214	TrGC	MC3ODBCO3H + OH → MC3CODBCO3	4.73E-11	Rickard and Pascoe (2009)
Aro215	TrGC	ACCOMECO3H + OH → ACCOMECO3	3.59E-12	Rickard and Pascoe (2009)
Aro216	TrGC	C5DIALO2 + HO_2 → C5DIALOOH	KRO2HO2*0.706*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro217	TrGC	C5DIALO2 + HO_2 → MALDIAL + CO + HO_2 + OH	KRO2HO2*0.706*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro218	TrGCN	C5DIALO2 + NO → MALDIAL + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro219	TrGCN	C5DIALO2 + NO_3 → MALDIAL + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro220	TrGC	C5DIALO2 → MALDIAL + CO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro221	TrGC	PHENOOH + OH → PHENO2	1.16E-10	Rickard and Pascoe (2009)
Aro222	TrGC	C6CO4DB + OH → CO + CO + HO_2 + CO + C33CO	7.70E-11	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro223	TrGC	C5CO2DCO3H + OH → C5CO2DBCO3	3.60E-11	Rickard and Pascoe (2009)
Aro224	TrGCN	NDNPHENOOH + OH → NDNPHENO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro225	TrGC	C615CO2O2 + HO_2 → C615CO2OOH	KRO2HO2*0.770*(1.-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro226	TrGC	C615CO2O2 + HO_2 → C5DICARB + CO + HO_2 + OH	KRO2HO2*0.770*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro227	TrGCN	C615CO2O2 + NO → C5DICARB + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro228	TrGCN	C615CO2O2 + NO_3 → C5DICARB + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro229	TrGC	C615CO2O2 → C5DICARB + CO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro230	TrGCN	BZEMUCPAN + OH → MALDIAL + CO + NO_2	4.05E-11	Rickard and Pascoe (2009)
Aro231	TrGCN	BZEMUCPAN → BZEMUCCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro232	TrGCN	BZBIPERNO3 + OH → BZOBIPEROH + NO_2	7.30E-11	Rickard and Pascoe (2009)
Aro233	TrGCN	HOC6H4NO2 + NO_3 → NPHEN1O + HNO_3	9.00E-14	Rickard and Pascoe (2009)
Aro234	TrGCN	HOC6H4NO2 + OH → NPHEN1O	9.00E-13	Rickard and Pascoe (2009)
Aro235	TrGCN	NDNPHENO2 + HO_2 → NDNPHENOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro236	TrGC	NDNPHENO2 + HO_2 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH	KRO2HO2*0.770*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro237	TrGCN	NDNPHENO2 + NO → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro238	TrGCN	NDNPHENO2 + NO_3 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro239	TrGCN	NDNPHENO2 → NC4DCO2H + HNO_3 + CO + CO + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro240	TrGC	PBZQCO + OH → C5CO2OHCO3	6.07E-11	Rickard and Pascoe (2009)
Aro241	TrGCN	CATECHOL + NO_3 → CATEC1O + HNO_3	9.9E-11	Rickard and Pascoe (2009)*
Aro242	TrGC	CATECHOL + O_3 → MALDALCO2H + $HCOCO_2H$ + HO_2 + OH	9.2E-18	Rickard and Pascoe (2009)
Aro243	TrGC	CATECHOL + OH → CATEC1O	1.0E-10	Rickard and Pascoe (2009)
Aro244	TrGC	C5COOHCO3H + OH → C5CO2OHCO3	8.01E-11	Rickard and Pascoe (2009)
Aro245	TrGCN	NCATECHOL + NO_3 → NNCATECO2	2.60E-12	Rickard and Pascoe (2009)
Aro246	TrGCN	NCATECHOL + OH → NCATECO2	3.47E-12	Rickard and Pascoe (2009)
Aro247	TrGC	C5CO2OHCO3 + HO_2 → C5COOHCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro248	TrGC	C5CO2OHCO3 + HO_2 → HOCOC4DIAL + HO_2 + CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro249	TrGCN	C5CO2OHCO3 + NO → HOCOC4DIAL + HO_2 + CO + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro250	TrGCN	C5CO2OHCO3 + NO_2 → C5CO2OHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro251	TrGCN	C5CO2OHCO3 + NO_3 → HOCOC4DIAL + HO_2 + CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro252	TrGC	C5CO2OHCO3 → HOCOC4DIAL + HO_2 + CO	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro253	TrGCN	BZEPOXMUC + NO_3 → BZEMUCCO3 + HNO_3	2*KNO3AL*2.75	Rickard and Pascoe (2009)
Aro254	TrGC	BZEPOXMUC + O_3 → EPXC4DIAL + .125 HCHO + .1125 $HCOCO_2H$ + .0675 GLYOX + .0675 H_2O_2 + .82 HO_2 + .57 OH + 1.265 CO	2.00E-18	Rickard and Pascoe (2009)*
Aro255	TrGC	BZEPOXMUC + OH → .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard and Pascoe (2009)
Aro256	TrGCN	NCATECO2 + HO_2 → NCATECOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro257	TrGC	NCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	KRO2HO2*0.770*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro258	TrGCN	NCATECO2 + NO → NC4DCO2H + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro259	TrGCN	NCATECO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro260	TrGCN	NCATECO2 → NC4DCO2H + $HCOCO_2H$ + HO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro261	TrGCN	NPHEN1OOH + OH → NPHEN1O2	9.00E-13	Rickard and Pascoe (2009)
Aro262	TrGCN	NPHENO2 + HO_2 → NPHENOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro263	TrGCN	NPHENO2 + HO_2 → MALDALCO2H + GLYOX + NO_2 + OH	KRO2HO2*0.770*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro264	TrGCN	NPHENO2 + NO → MALDALCO2H + GLYOX + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro265	TrGCN	NPHENO2 + NO_3 → MALDALCO2H + GLYOX + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro266	TrGCN	NPHENO2 → MALDALCO2H + GLYOX + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro267	TrGC	BENZENE + OH → .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO_2 + .53 PHENOL + .53 HO_2	2.3E-12*EXP(-190/TEMP)	Rickard and Pascoe (2009)*
Aro268	TrGCN	C5CO2OHPAN + OH → HOCOC4DIAL + CO + CO + NO_2	7.66E-11	Rickard and Pascoe (2009)
Aro269	TrGCN	C5CO2OHPAN → C5CO2OHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro270	TrGCN	CATEC1O + NO_2 → NCATECHOL	2.08E-12	Rickard and Pascoe (2009)
Aro271	TrGC	CATEC1O + O_3 → CATEC1O2	2.86E-13	Rickard and Pascoe (2009)
Aro272	TrGC	BZEMUCCO + OH → EPXDLCO3 + GLYOX	9.20E-11	Rickard and Pascoe (2009)
Aro273	TrGCN	NNCATECO2 + HO_2 → NNCATECOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro274	TrGCN	NNCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	KRO2HO2*0.770*(rchohch2o2_oh)	Rickard and Pascoe (2009)*
Aro275	TrGCN	NNCATECO2 + NO → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro276	TrGCN	NNCATECO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro277	TrGCN	NNCATECO2 → NC4DCO2H + $HCOCO_2H$ + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro278	TrGC	BZEMUCCO2H + OH → C5DIALO2	4.06E-11	Rickard and Pascoe (2009)
Aro279	TrGCN	NNCATECOOH + OH → NNCATECO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro280	TrGCN	NPHEN1O + NO_2 → DNPHEN	2.08E-12	Rickard and Pascoe (2009)
Aro281	TrGCN	NPHEN1O + O_3 → NPHEN1O2	2.86E-13	Rickard and Pascoe (2009)
Aro282	TrGCN	DNPHEN + NO_3 → NDNPHENO2	2.25E-15	Rickard and Pascoe (2009)
Aro283	TrGCN	DNPHEN + OH → DNPHENO2	3.00E-14	Rickard and Pascoe (2009)
Aro284	TrGCN	PHENOL + NO_3 → .742 C6H5O + .742 HNO_3 + .258 NPHENO2	3.8E-12	Rickard and Pascoe (2009)*
Aro285	TrGC	PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 HO_2 + .14 PHENO2	4.7E-13*EXP(1220/TEMP)	Rickard and Pascoe (2009)*
Aro286	TrGCN	PBZQONE + NO_3 → NBZQO2	3.00E-13	Rickard and Pascoe (2009)
Aro287	TrGC	PBZQONE + OH → PBZQO2	4.6E-12	Rickard and Pascoe (2009)
Aro288	TrGC	PHENO2 + HO_2 → PHENOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro289	TrGC	PHENO2 + HO_2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH	KRO2HO2*0.770*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro290	TrGCN	PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro291	TrGCN	PHENO2 + NO_3 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro292	TrGC	PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro293	TrGC	C615CO2OOH + OH → C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
Aro294	TrGC	C5CO2DBCO3 + HO_2 → C5CO2DCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro295	TrGC	C5CO2DBCO3 + HO_2 → $CH_3C(O)OO$ + C33CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro296	TrGCN	C5CO2DBCO3 + NO → $CH_3C(O)OO$ + C33CO + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro297	TrGCN	C5CO2DBCO3 + NO_2 → C5CO2DBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro298	TrGCN	C5CO2DBCO3 + NO_3 → $CH_3C(O)OO$ + C33CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro299	TrGC	C5CO2DBCO3 → $CH_3C(O)OO$ + C33CO	KRO2AP*RO2	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro300	TrGCN	NPHEN1O2 + HO_2 → NPHEN1OOH	KRO2HO2*0.770	Rickard and Pascoe (2009)
Aro301	TrGCN	NPHEN1O2 + NO → NPHEN1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro302	TrGCN	NPHEN1O2 + NO_2 → NPHEN1O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro303	TrGCN	NPHEN1O2 + NO_3 → NPHEN1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro304	TrGCN	NPHEN1O2 → NPHEN1O	KRO2sRO2*RO2	Rickard and Pascoe (2009)
Aro305	TrGCN	NPHENOOH + OH → NPHENO2	1.07E-10	Rickard and Pascoe (2009)
Aro306	TrGCN	C6H5O + NO_2 → HOC6H4NO2	2.08E-12	Rickard and Pascoe (2009)*
Aro307	TrGC	C6H5O + O_3 → C6H5O2	2.86E-13	Rickard and Pascoe (2009)
Aro308	TrGCN	NCATECOOH + OH → NCATECO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro309	TrGC	PBZQOOH + OH → PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)
Aro310	TrGC	PBZQO2 + HO_2 → PBZQOOH	KRO2HO2*0.770*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro311	TrGC	PBZQO2 + HO_2 → C5CO2OHCO3 + OH	KRO2HO2*0.770*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
Aro312	TrGCN	PBZQO2 + NO → C5CO2OHCO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro313	TrGCN	PBZQO2 + NO_3 → C5CO2OHCO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro314	TrGC	PBZQO2 → C5CO2OHCO3	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro315	TrGC	BZOBIPEROH + OH → MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
Aro316	TrGCN	DNPHENO2 + HO_2 → DNPHENOOH	KRO2HO2*0.770*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro317	TrGCN	DNPHENO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	KRO2HO2*0.770*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro318	TrGCN	DNPHENO2 + NO → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro319	TrGCN	DNPHENO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro320	TrGCN	DNPHENO2 → NC4DCO2H + $HCOCO_2H$ + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro321	TrGC	BZBIPEROOH + OH → BZOBIPEROH + OH	9.77E-11	Rickard and Pascoe (2009)
Aro322	TrGC	BZEMUCO2 + HO_2 → BZEMUCOOH	KRO2HO2*0.770*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro323	TrGC	BZEMUCO2 + HO_2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + OH	KRO2HO2*0.770*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
Aro324	TrGCN	BZEMUCO2 + NO → BZEMUCNO3	KRO2NO*0.105	Rickard and Pascoe (2009)
Aro325	TrGCN	BZEMUCO2 + NO → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + NO_2	KRO2NO*0.895	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro326	TrGCN	BZEMUCO2 + NO_3 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro327	TrGC	BZEMUCO2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro328	TrGCN	C5CO2DBPAN + OH → C33CO + CH_3CHO + NO_2	3.28E-11	Rickard and Pascoe (2009)
Aro329	TrGCN	C5CO2DBPAN → C5CO2DBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro330	TrGCN	NBZQOOH + OH → NBZQO2	6.68E-11	Rickard and Pascoe (2009)
Aro331	TrGC	CATEC1OOH + OH → CATEC1O2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro332	TrGC	C6125CO + OH → C5CO14O2 + CO	6.45E-11	Rickard and Pascoe (2009)
Aro333	TrGCN	NBZQO2 + HO_2 → NBZQOOH	KRO2HO2*0.770*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro334	TrGCN	NBZQO2 + HO_2 → C6CO4DB + NO_2 + OH	KRO2HO2*0.770*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro335	TrGCN	NBZQO2 + NO → C6CO4DB + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro336	TrGCN	NBZQO2 + NO_3 → C6CO4DB + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro337	TrGCN	NBZQO2 → C6CO4DB + NO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro338	TrGCN	DNPHENOOH + OH → DNPHENO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro339	TrGC	CATEC1O2 + HO_2 → CATEC1OOH	KRO2HO2*0.770	Rickard and Pascoe (2009)
Aro340	TrGCN	CATEC1O2 + NO → CATEC1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro341	TrGCN	CATEC1O2 + NO_2 → CATEC1O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro342	TrGCN	CATEC1O2 + NO_3 → CATEC1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro343	TrGC	CATEC1O2 → CATEC1O	8.80E-13*RO2	Rickard and Pascoe (2009)
Aro344	TrGC	BZEMUCCO3H + OH → BZEMUCCO3	4.37E-11	Rickard and Pascoe (2009)
Aro345	TrGC	C6H5OOH + OH → C6H5O2	3.60E-12	Rickard and Pascoe (2009)
Aro346	TrGC	BZEMUCOOH + OH → BZEMUCCO + OH	1.31E-10	Rickard and Pascoe (2009)
Aro347	TrGC	BZEMUCCO3 + HO_2 → BZEMUCCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro348	TrGC	BZEMUCCO3 + HO_2 → BZEMUCCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro349	TrGC	BZEMUCCO3 + HO_2 → C5DIALO2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro350	TrGCN	BZEMUCCO3 + NO → C5DIALO2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro351	TrGCN	BZEMUCCO3 + NO_2 → BZEMUCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro352	TrGCN	BZEMUCCO3 + NO_3 → C5DIALO2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro353	TrGC	BZEMUCCO3 → C5DIALO2	1.00E-11*RO2	Rickard and Pascoe (2009)*
Aro354	TrGC	C6H5O2 + HO_2 → C6H5OOH	KRO2HO2*0.770	Rickard and Pascoe (2009)
Aro355	TrGCN	C6H5O2 + NO → C6H5O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro356	TrGCN	C6H5O2 + NO_2 → C6H5O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro357	TrGCN	C6H5O2 + NO_3 → C6H5O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro358	TrGC	C6H5O2 → C6H5O	KRO2sRO2*RO2	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro359	TrGC	BZEMUCOH + OH → BZEMUCCO + HO_2	8.23E-11	Rickard and Pascoe (2009)
Aro360	TrGCN	BZEMUCNO3 + OH → BZEMUCCO + NO_2	4.38E-11	Rickard and Pascoe (2009)
Aro361	TrGC	TOLUENE + OH → .07 C6H5CH2O2 + .07 $PTOL_C$6H5CH2O2 + .18 CRESOL + .18 $PTOL_C$RESOL + .18 HO_2 + .65 TLBIPERO2 + .65 $PTOL_T$LBIPERO2 + .10 TLEPOXMUC + .10 $PTOL_T$LEPOXMUC + .10 HO_2	1.8E-12*EXP(340/TEMP)	Rickard and Pascoe (2009)*
Aro362	TrGC	BZBIPERO2 + HO_2 → BZBIPEROOH	KRO2HO2*0.770	Rickard and Pascoe (2009)
Aro363	TrGCN	BZBIPERO2 + NO → BZBIPERNO3	KRO2NO*0.082	Rickard and Pascoe (2009)
Aro364	TrGCN	BZBIPERO2 + NO → NO_2 + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	KRO2NO*0.918	Rickard and Pascoe (2009)*
Aro365	TrGCN	BZBIPERO2 + NO_3 → NO_2 + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	KRO2NO3	Rickard and Pascoe (2009)*
Aro366	TrGC	BZBIPERO2 → GLYOX + HO_2 + BZFUONE	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro367	TrGC	C6H5CH2O2 + HO_2 → C6H5CH2OOH	1.5E-13*EXP(1310/TEMP)	Rickard and Pascoe (2009)
Aro368	TrGCN	C6H5CH2O2 + NO → C6H5CH2NO3	KRO2NO*0.105	Rickard and Pascoe (2009)*
Aro369	TrGCN	C6H5CH2O2 + NO → BENZAL + HO_2 + NO_2	KRO2NO*0.985	Rickard and Pascoe (2009)*
Aro370	TrGCN	C6H5CH2O2 + NO_3 → BENZAL + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro371	TrGC	C6H5CH2O2 → BENZAL + HO_2	2*(KCH3O2*2.4E-14*EXP(1620/TEMP))**0.5*RO2	Rickard and Pascoe (2009)*
Aro372	TrGCN	CRESOL + NO_3 → .103 CRESO2 + .103 HNO_3 + .506 NCRESO2 + .391 TOL1O + .391 HNO_3	1.4E-11	Rickard and Pascoe (2009)*
Aro373	TrGC	CRESOL + OH → .2 CRESO2 + .727 MCATECHOL + .727 HO_2 + .073 TOL1O	4.65E-11	Rickard and Pascoe (2009)*
Aro374	TrGC	TLBIPERO2 + HO_2 → TLBIPEROOH	KRO2HO2*0.820	Rickard and Pascoe (2009)
Aro375	TrGCN	TLBIPERO2 + NO → NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KRO2NO*0.889	Rickard and Pascoe (2009)*
Aro376	TrGCN	TLBIPERO2 + NO → TLBIPERNO3	KRO2NO*0.111	Rickard and Pascoe (2009)
Aro377	TrGCN	TLBIPERO2 + NO_3 → NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KRO2NO3	Rickard and Pascoe (2009)*
Aro378	TrGC	TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	8.80E-13*RO2	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro379	TrGCN	TLEPOXMUC + NO_3 → TLEMUCCO3 + HNO_3	KNO3AL*2.75	Rickard and Pascoe (2009)
Aro380	TrGC	TLEPOXMUC + O_3 → EPXC4DIAL + .125 CH_3CHO + .695 $CH_3C(O)OO$ + .57 CO + .57 OH + .125 HO_2 +.1125 CH3COCO2H + .0675 MGLYOX + .0675 H_2O_2	5.00E-18	Rickard and Pascoe (2009)*
Aro381	TrGC	TLEPOXMUC + OH → .31 TLEMUCCO3 + .69 TLEMUCO2	7.99E-11	Rickard and Pascoe (2009)*
Aro382	TrGC	C6H5CH2OOH + OH → BENZAL + OH	2.05E-11	Rickard and Pascoe (2009)
Aro383	TrGCN	C6H5CH2NO3 + OH → BENZAL + NO_2	6.03E-12	Rickard and Pascoe (2009)
Aro384	TrGCN	BENZAL + NO_3 → C6H5CO3 + HNO_3	2.40E-15	Rickard and Pascoe (2009)
Aro385	TrGC	BENZAL + OH → C6H5CO3	5.9E-12*EXP(225/TEMP)	Rickard and Pascoe (2009)
Aro386	TrGC	CRESO2 + HO_2 → CRESOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro387	TrGC	CRESO2 + HO_2 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro388	TrGCN	CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro389	TrGCN	CRESO2 + NO_3 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro390	TrGC	CRESO2 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro391	TrGCN	NCRESO2 + HO_2 → NCRESOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro392	TrGCN	NCRESO2 + HO_2 → C5CO14OH + GLYOX + NO_2 + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro393	TrGCN	NCRESO2 + NO → C5CO14OH + GLYOX + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro394	TrGCN	NCRESO2 + NO_3 → C5CO14OH + GLYOX + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro395	TrGCN	NCRESO2 → C5CO14OH + GLYOX + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro396	TrGCN	TOL1O + NO_2 → TOL1OHNO2	2.08E-12	Rickard and Pascoe (2009)*
Aro397	TrGC	TOL1O + O_3 → OXYL1O2	2.86E-13	Rickard and Pascoe (2009)
Aro398	TrGCN	MCATECHOL + NO_3 → MCATEC1O + HNO_3	1.7E-10*1.0	Rickard and Pascoe (2009)
Aro399	TrGC	MCATECHOL + O_3 → MC3ODBCO2H + $HCOCO_2H$ + HO_2 + OH	2.8E-17	Rickard and Pascoe (2009)*
Aro400	TrGC	MCATECHOL + OH → MCATEC1O	2.0E-10*1.0	Rickard and Pascoe (2009)
Aro401	TrGC	TLBIPEROOH + OH → TLOBIPEROH + OH	9.64E-11	Rickard and Pascoe (2009)
Aro402	TrGCN	TLBIPERNO3 + OH → TLOBIPEROH + NO_2	7.16E-11	Rickard and Pascoe (2009)
Aro403	TrGC	TLOBIPEROH + OH → C5CO14O2 + GLYOX	7.99E-11	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro404	TrGC	TLEMUCCO3 + HO_2 → C615CO2O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro405	TrGC	TLEMUCCO3 + HO_2 → TLEMUCCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)*
Aro406	TrGCN	TLEMUCCO3 + HO_2 → TLEMUCCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)*
Aro407	TrGCN	TLEMUCCO3 + NO → C615CO2O2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro408	TrGCN	TLEMUCCO3 + NO_2 → TLEMUCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro409	TrGCN	TLEMUCCO3 + NO_3 → C615CO2O2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro410	TrGC	TLEMUCCO3 → C615CO2O2	KRO2AP*RO2	Rickard and Pascoe (2009)*
Aro411	TrGC	TLEMUCO2 + HO_2 → TLEMUCOOH	KRO2HO2*0.820*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro412	TrGC	TLEMUCO2 + HO_2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH	KRO2HO2*0.820*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
Aro413	TrGCN	TLEMUCO2 + NO → TLEMUCNO3	KRO2NO*0.105	Rickard and Pascoe (2009)
Aro414	TrGCN	TLEMUCO2 + NO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + NO_2	KRO2NO*0.985	Rickard and Pascoe (2009)*
Aro415	TrGCN	TLEMUCO2 + NO_3 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro416	TrGCN	TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro417	TrGC	C6H5CO3 + HO_2 → C6H5CO3H	KAPHO2*0.065	Roth et al. (2010)*
Aro418	TrGC	C6H5CO3 + HO_2 → C6H5O2 + OH	KAPHO2*0.20	Roth et al. (2010)*
Aro419	TrGC	C6H5CO3 + HO_2 → PHCOOH + O_3	KAPHO2*0.15	Roth et al. (2010)*
Aro420	TrGCN	C6H5CO3 + NO → C6H5O2 + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro421	TrGCN	C6H5CO3 + NO_2 → PBZN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro422	TrGCN	C6H5CO3 + NO_3 → C6H5O2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro423	TrGC	C6H5CO3 → C6H5O2	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro424	TrGC	CRESOOH + OH → CRESO2	1.15E-10	Rickard and Pascoe (2009)
Aro425	TrGCN	NCRESOOH + OH → NCRESO2	1.07E-10	Rickard and Pascoe (2009)
Aro426	TrGCN	TOL1OHNO2 + NO_3 → NCRES1O + HNO_3	3.13E-13*1.0	Rickard and Pascoe (2009)
Aro427	TrGCN	TOL1OHNO2 + OH → NCRES1O	2.8E-12	Rickard and Pascoe (2009)
Aro428	TrGC	OXYL1O2 + HO_2 → OXYL1OOH	KRO2HO2*0.820	Rickard and Pascoe (2009)
Aro429	TrGCN	OXYL1O2 + NO → TOL1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro430	TrGCN	OXYL1O2 + NO_2 → TOL1O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro431	TrGCN	OXYL1O2 + NO_3 → TOL1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro432	TrGC	OXYL1O2 → TOL1O	KRO2sRO2*RO2	Rickard and Pascoe (2009)
Aro433	TrGCN	MCATEC1O + NO_2 → MNCATECH	2.08E-12	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro434	TrGC	MCATEC1O + O_3 → MCATEC1O2	2.86E-13	Rickard and Pascoe (2009)
Aro435	TrGCAro	C4MDIAL + NO_3 → MC3CODBCO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
Aro436	TrGCAro	C4MDIAL + NO_3 → C3MCODBCO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
Aro437	TrGCN	C4MDIAL + O_3 → .445 OH + .445 CO + .445 $CH_3C(O)OO$ + .055 MGLYOX + .055 H_2O_2 + .5 GLYOX + .5 MGLYOX + .0343 $HCOCO_2H$ + .0206 GLYOX + .0206 H_2O_2 + .445 OH + .445 HO_2 + .445 CO + .445 CO	5.00E-18	Rickard and Pascoe (2009)
Aro438	TrGC	C4MDIAL + OH → .385 C3MCODBCO3 + .23 C4M2ALOHO2 + .385 MC3CODBCO3	4.41E-11	Rickard and Pascoe (2009)
Aro439	TrGC	TLEMUCCO2H + OH → C615CO2O2	5.98E-11	Rickard and Pascoe (2009)
Aro440	TrGC	TLEMUCCO3H + OH → TLEMUCCO3	6.29E-11	Rickard and Pascoe (2009)
Aro441	TrGCN	TLEMUCPAN + OH → C5DICARB + CO + NO_2	5.96E-11	Rickard and Pascoe (2009)
Aro442	TrGCN	TLEMUCPAN → TLEMUCCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro443	TrGC	TLEMUCOOH + OH → TLEMUCCO + OH	7.04E-11	Rickard and Pascoe (2009)
Aro444	TrGCN	TLEMUCNO3 + OH → TLEMUCCO + NO_2	3.06E-11	Rickard and Pascoe (2009)
Aro445	TrGC	TLEMUCCO + OH → $CH_3C(O)OO$ + EPXC4DIAL + CO	4.06E-11	Rickard and Pascoe (2009)
Aro446	TrGC	C6H5CO3H + OH → C6H5CO3	4.66E-12	Rickard and Pascoe (2009)
Aro447	TrGC	PHCOOH + OH → C6H5O2	1.10E-12	Rickard and Pascoe (2009)
Aro448	TrGCN	PBZN + OH → C6H5OOH + CO + NO_2	1.06E-12	Rickard and Pascoe (2009)
Aro449	TrGCN	PBZN → C6H5CO3 + NO_2	k_PAN_M*0.67	Rickard and Pascoe (2009)*
Aro450	TrGCN	PTLQONE + NO_3 → NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
Aro451	TrGC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard and Pascoe (2009)
Aro452	TrGCN	NCRES1O + NO_2 → DNCRES	2.08E-12	Rickard and Pascoe (2009)
Aro453	TrGCN	NCRES1O + O_3 → NCRES1O2	2.86E-13	Rickard and Pascoe (2009)
Aro454	TrGC	OXYL1OOH + OH → OXYL1O2	4.65E-11	Rickard and Pascoe (2009)
Aro455	TrGCN	MNCATECH + NO_3 → MNNCATECO2	5.03E-12	Rickard and Pascoe (2009)
Aro456	TrGCN	MNCATECH + OH → MNCATECO2	6.83E-12	Rickard and Pascoe (2009)
Aro457	TrGC	MCATEC1O2 + HO_2 → MCATEC1OOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro458	TrGC	MCATEC1O2 + HO_2 → MCATEC1O + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro459	TrGCN	MCATEC1O2 + NO → MCATEC1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro460	TrGCN	MCATEC1O2 + NO_2 → MCATEC1O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro461	TrGCN	MCATEC1O2 + NO_3 → MCATEC1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro462	TrGC	MCATEC1O2 → MCATEC1O	8.80E-13*RO2	Rickard and Pascoe (2009)
Aro463	TrGCN	NPTLQO2 + HO_2 → NPTLQOOH	KRO2HO2*0.820*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro464	TrGCN	NPTLQO2 + HO_2 → C7CO4DB + NO_2 + OH	KRO2HO2*0.820*rcoch2o2_oh	Rickard and Pascoe (2009)*
Aro465	TrGCN	NPTLQO2 + NO → C7CO4DB + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro466	TrGCN	NPTLQO2 + NO_3 → C7CO4DB + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro467	TrGCN	NPTLQO2 → C7CO4DB + NO_2	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro468	TrGC	PTLQO2 + HO_2 → PTLQOOH	KRO2HO2*0.820*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
Aro469	TrGC	PTLQO2 + HO_2 → C6CO2OHCO3 + OH	KRO2HO2*0.820*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
Aro470	TrGCN	PTLQO2 + NO → C6CO2OHCO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro471	TrGCN	PTLQO2 + NO_3 → C6CO2OHCO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro472	TrGC	PTLQO2 → C6CO2OHCO3	8.80E-13*RO2	Rickard and Pascoe (2009)*
Aro473	TrGCN	DNCRES + NO_3 → NDNCRESO2	7.83E-15	Rickard and Pascoe (2009)
Aro474	TrGCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard and Pascoe (2009)
Aro475	TrGCN	NCRES1O2 + HO_2 → NCRES1OOH	KRO2HO2*0.820	Rickard and Pascoe (2009)
Aro476	TrGCN	NCRES1O2 + NO → NCRES1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
Aro477	TrGCN	NCRES1O2 + NO_2 → NCRES1O + NO_3	KPHENO2NO2	Jagiella and Zabel (2007)*
Aro478	TrGCN	NCRES1O2 + NO_3 → NCRES1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
Aro479	TrGCN	NCRES1O2 → NCRES1O	KRO2sRO2*RO2	Rickard and Pascoe (2009)
Aro480	TrGCN	MNNCATECO2 + HO_2 → MNNCATCOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro481	TrGCN	MNNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro482	TrGCN	MNNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro483	TrGCN	MNNCATECO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro484	TrGCN	MNNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)
Aro485	TrGCN	MNCATECO2 + HO_2 → MNCATECOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro486	TrGCN	MNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro487	TrGCN	MNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro488	TrGCN	MNCATECO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro489	TrGCN	MNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + HO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro490	TrGC	MCATEC1OOH + OH → MCATEC1O2	2.05E-10	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro491	TrGCN	C3MCODBPANN + OH → MGLYOX + CO + CO + NO_2	4.37E-11	Rickard and Pascoe (2009)
Aro492	TrGCN	C3MCODBPANN → C3MCODBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro493	TrGC	MCOCOMOXO2 + HO_2 → MCOCOMOOOH	KRO2HO2*0.625*(1-.4)	Rickard and Pascoe (2009)*
Aro494	TrGC	MCOCOMOXO2 + HO_2 → HCHO + $CH_3C(O)OO$ + OH	KRO2HO2*0.625*.4	Rickard and Pascoe (2009)*
Aro495	TrGCN	MCOCOMOXO2 + NO → HCHO + $CH_3C(O)OO$ + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro496	TrGCN	MCOCOMOXO2 + NO_3 → HCHO + $CH_3C(O)OO$ + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro497	TrGC	MCOCOMOXO2 → HCHO + $CH_3C(O)OO$	KRO2pORO2*RO2	Rickard and Pascoe (2009)*
Aro498	TrGCN	NPTLQOOH + OH → NPTLQO2	8.56E-11	Rickard and Pascoe (2009)
Aro499	TrGC	PTLQOOH + OH → PTLQCO + OH	1.42E-10	Rickard and Pascoe (2009)
Aro500	TrGC	PTLQCO + OH → C6CO2OHCO3	7.95E-11	Rickard and Pascoe (2009)
Aro501	TrGCN	NDNCRESO2 + HO_2 → NDNCRESOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro502	TrGCN	NDNCRESO2 + HO_2 → NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro503	TrGCN	NDNCRESO2 + NO → NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro504	TrGCN	NDNCRESO2 + NO_3 → NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro505	TrGCN	NDNCRESO2 → NC4MDCO2HN + HNO_3 + CO + CO + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro506	TrGCN	DNCRESO2 + HO_2 → DNCRESOOH	KRO2HO2*0.820*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro507	TrGCN	DNCRESO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	KRO2HO2*0.820*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro508	TrGCN	DNCRESO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
Aro509	TrGCN	DNCRESO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
Aro510	TrGCN	DNCRESO2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2	8.00E-13*RO2	Rickard and Pascoe (2009)*
Aro511	TrGCN	NCRES1OOH + OH → NCRES1O2	1.53E-12	Rickard and Pascoe (2009)
Aro512	TrGC	MNNCATCOOH + OH → MNNCATECO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro513	TrGCN	MNCATECOOH + OH → MNCATECO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro514	TrGCN	NO_3 + CO23C3CHO → $CH_3C(O)OO$ + CO + CO + HNO_3	KNO3AL*4.0	Rickard and Pascoe (2009)
Aro515	TrGC	OH + CO23C3CHO → $CH_3C(O)OO$ + CO + CO	1.23E-11	Rickard and Pascoe (2009)
Aro516	TrGC	C7CO4DB + OH → CO + CO + $CH_3C(O)OO$ + C33CO	9.58E-11	Rickard and Pascoe (2009)

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

reaction	rate coefficient	reference		
Aro517	TrGC	C6CO2OHCO3 + HO_2 → C5134CO2OH + HO_2 + CO + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
Aro518	TrGC	C6CO2OHCO3 + HO_2 → C6COOHCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)*
Aro519	TrGCN	C6CO2OHCO3 + NO → C5134CO2OH + HO_2 + CO + NO_2	KAPNO	Rickard and Pascoe (2009)
Aro520	TrGCN	C6CO2OHCO3 + NO_2 → C6CO2OHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
Aro521	TrGCN	C6CO2OHCO3 + NO_3 → C5134CO2OH + HO_2 + CO + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
Aro522	TrGC	C6CO2OHCO3 → C5134CO2OH + HO_2 + CO	KRO2AP*RO2	Rickard and Pascoe (2009)
Aro523	TrGCN	NDNCRESOOH + OH → NDNCRESO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro524	TrGCN	DNCRESOOH + OH → DNCRESO2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009)
Aro525	TrGC	C6COOHCO3H + OH → C6CO2OHCO3	9.29E-11	Rickard and Pascoe (2009)
Aro526	TrGCN	C6CO2OHPAN + OH → C5134CO2OH + CO + CO + NO_2	8.96E-11	Rickard and Pascoe (2009)
Aro527	TrGCN	C6CO2OHPAN → C6CO2OHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
Aro528	TrGC	LXYL + OH → TLEPOXMUC + HO_2 + $PXYL_T$LEPOXMUC + LCARBON	0.401E-11	Rickard and Pascoe (2009)*
Aro529	TrGC	LXYL + OH → C6H5CH2O2 + $PXYL_C$6H5CH2O2 + LCARBON	0.101E-11	Rickard and Pascoe (2009)*
Aro530	TrGC	LXYL + OH → CRESOL + $PXYL_C$RESOL + LCARBON	0.261E-11	Rickard and Pascoe (2009)*
Aro531	TrGC	LXYL + OH → TLBIPERO2 + HO_2 + $PXYL_T$LBIPERO2 + LCARBON	0.932E-11	Rickard and Pascoe (2009)*
Aro532	TrGCN	LXYL + NO_3 → C6H5CH2O2 + HNO_3 + $PXYL_C$6H5CH2O2 + LCARBON	3.9E-16	Rickard and Pascoe (2009)*
Aro533	TrGC	LTMB + OH → TLEPOXMUC + HO_2 + $PTMB_T$LEPOXMUC + 2 LCARBON	0.827E-11	Rickard and Pascoe (2009)*
Aro534	TrGC	LTMB + OH → C6H5CH2O2 + $PTMB_C$6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard and Pascoe (2009)*
Aro535	TrGC	LTMB + OH → CRESOL + $PTMB_C$RESOL + 2 LCARBON	0.141E-11	Rickard and Pascoe (2009)*
Aro536	TrGC	LTMB + OH → TLBIPERO2 + HO_2 + $PTMB_T$LBIPERO2 + 2 LCARBON	2.917E-11	Rickard and Pascoe (2009)*
Aro537	TrGCN	LTMB + NO_3 → C6H5CH2O2 + HNO_3 + $PTMB_C$6H5CH2O2 + 2 LCARBON	1.52E-15	Rickard and Pascoe (2009)*

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

reaction	rate coefficient	reference		
Aro538	TrGC	EBENZ + OH → .10 TLEPOXMUC + .07 C6H5CH2O2 + .18 CRESOL + .65 TLBIPERO2 + 0.28 HO_2 + LCARBON	7.00E-12	Rickard and Pascoe (2009)*
Aro539	TrGCN	EBENZ + NO_3 → C6H5CH2O2 + HNO_3 + LCARBON	1.20E-16	Rickard and Pascoe (2009)*
Aro540	TrGC	HAROM + OH → .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + 0.18 HO_2 + 4 LCARBON	5.67E-11	Rickard and Pascoe (2009)*
Aro541	TrGCN	HAROM + NO_3 → C6H5CH2O2 + HNO_3 + 4 LCARBON	2.60E-15	Rickard and Pascoe (2009)*
Aro542	TrGCN	NO_3 + STYRENE → NSTYRENO2	1.50E-12	Rickard and Pascoe (2009)
Aro543	TrGC	O_3 + STYRENE → .545 HCHO + .1 BENZENE + .28 C6H5O2 + .56 CO + .36 OH + .28 HO_2 + .075 PHCOOH + .545 BENZAL + .09 H_2O_2 + .075 HCOOH	1.70E-17	Rickard and Pascoe (2009)*
Aro544	TrGC	OH + STYRENE → STYRENO2	5.80E-11	Rickard and Pascoe (2009)
Aro545	TrGCN	NSTYRENO2 + HO_2 → NSTYRENOOH	KRO2HO2*0.859	Rickard and Pascoe (2009)
Aro546	TrGCN	NSTYRENO2 + NO → NO_2 + NO_2 + HCHO + BENZAL	KRO2NO	Rickard and Pascoe (2009)*
Aro547	TrGCN	NSTYRENO2 + NO_3 → NO_2 + NO_2 + HCHO + BENZAL	KRO2NO3	Rickard and Pascoe (2009)*
Aro548	TrGCN	NSTYRENO2 → NO_2 + HCHO + BENZAL	KRO2sRO2*RO2	Rickard and Pascoe (2009)*
Aro549	TrGCN	OH + NSTYRENOOH → NSTYRENO2	6.16E-11	Rickard and Pascoe (2009)
Aro550	TrGC	STYRENO2 + HO_2 → STYRENOOH	KRO2HO2*0.859*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
Aro551	TrGCN	STYRENO2 + HO_2 → NO_2 + OH + HCHO + BENZAL	KRO2HO2*0.859*rchohch2o2_oh	Rickard and Pascoe (2009)*
Aro552	TrGCN	STYRENO2 + NO → NO_2 + HO_2 + HCHO + BENZAL	KRO2NO	Rickard and Pascoe (2009)*
Aro553	TrGCN	STYRENO2 + NO_3 → NO_2 + HO_2 + HCHO + BENZAL	KRO2NO3	Rickard and Pascoe (2009)*
Aro554	TrGC	STYRENO2 → HO_2 + HCHO + BENZAL	KRO2sRO2*RO2	Rickard and Pascoe (2009)*
Aro555	TrGC	OH + STYRENOOH → STYRENO2	6.16E-11	Rickard and Pascoe (2009)

Aromatic gas phase reactions notes:

Aro003: MGLYOX + GLYOX + HO2 from KDEC substitution

Aro004: MGLYOX + GLYOX + HO2 from KDEC substitution

Aro005: permutation reaction (minor channels removed)

Aro011: KDEC C3DIALO → GLYOX + CO + HO2

Aro012: KDEC C3DIALO → GLYOX + CO + HO2

Aro013: permutation reaction (minor channels removed)

Aro014: rco3_oh updated

Aro015: rco3_ooh+rco3_o3 updated

Aro029: KDEC NC4DCO2→ MALANHY + NO2

Aro033: rco3_o3 updated

Aro034: rco3_ooh updated

Aro035: rco3_oh updated + KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO

Aro036: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO

Aro038: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO

Aro039: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO

Aro041: KDEC BZFUONOOA → .5 BZFUONOO + .5 CO + .5 HCOCH2O2 + .5 OH and BZFUONOO → .625 CO14O3CO2H + .375 CO14O3CHO + .375 H2O2
Aro046: updated `rco3_oh`
Aro047: updated `rco3_o3`
Aro048: updated `rco3_ooh`
Aro052: Only major channel taken
Aro055: KDEC: GLYOOA → .125 HCHO + .18 GLYOO + 0.82 HO2 + .57 OH + 1.265 CO and H2O substitution GLYOO → .625 HCOCO2H + .375 GLYOX + .375 H2O2
Aro056: merged equations

Aro062: KDEC MALANHYO → HCOCOHCO3
Aro063: KDEC MALANHYO → HCOCOHCO3
Aro064: Only major channel taken and KDEC MALANHYO → HCOCOHCO3

Aro069: KDEC NBZFUO → .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2
Aro070: KDEC NBZFUO → .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2
Aro071: KDEC NBZFUO → .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2 and RO2 Only major channel taken
Aro072: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO

Aro077: KDEC MECOACETO → CH3CO3 + HCHO
Aro078: KDEC MECOACETO → CH3CO3 + HCHO
Aro079: KDEC MECOACETO → CH3CO3 + HCHO

Aro085: KDEC BZFUO → CO14O3CHO + HO2
Aro086: KDEC BZFUO → CO14O3CHO + HO2
Aro087: KDEC BZFUO → CO14O3CHO + HO2 and Only major channel taken

Aro093: KDEC MALDIALO → GLYOX + GLYOX + HO2
Aro094: KDEC MALDIALO → GLYOX + GLYOX + HO2
Aro095: KDEC MALDIALO → GLYOX + GLYOX + HO2 and Only major channel taken
Aro096: KDEC NC4MDCO2 → MMALANHY + NO2

Aro101: KDEC NTLFUO → ACCOMECHO + NO2
Aro102: KDEC NTLFUO → ACCOMECHO + NO2
Aro103: KDEC NTLFUO → ACCOMECHO
Aro105: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2 and updated `rco3_oh`
Aro106: updated `rco3_o3`
Aro107: updated `rco3_ooh`
Aro108: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2
Aro110: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2
Aro111: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2 and Only major channel taken

Aro116: updated `rco3_ooh`+ `rco3_o3`
Aro117: updated `rco3_oh`

Aro125: KDEC NPXYFUO → C23O3CCHO + NO2
Aro126: KDEC NPXYFUO → C23O3CCHO + NO2
Aro127: KDEC NPXYFUO → C23O3CCHO + NO2

Aro130: KDEC MMALANHYO→CO2H3CO3
Aro131: KDEC MMALANHYO→CO2H3CO3
Aro132: KDEC MMALANHYO→CO2H3CO3 and Only major channel taken
Aro138: updated `rco3_oh` and KDEC C5CO14CO2 →.83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO
Aro139: updated `rco3_o3`
Aro140: updated `rco3_ooh`
Aro141: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO
Aro143: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO
Aro144: KDEC C5CO14CO2 →.83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO and Only major channel taken
Aro148: KDEC C5CO14CO2 → .83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO

Aro151: KDEC NPXYFUO → C23O3CCHO + NO2
Aro152: KDEC NPXYFUO → C23O3CCHO + NO2
Aro153: KDEC NPXYFUO → C23O3CCHO + NO2
//1. original //C5DICARB + O3 = GLYOX + MGLOOB : 2.00E-18*0.5 ;
//1. KDEC C5DICARB + O3 = GLYOX + .125 CH3CHO + .695 CH3CO3 + .57 CO + .57 OH + .125 HO2 +.18 MGLOO : 2.00E-18*0.5 ;
//2. original //C5DICARB + O3 = MGLYOX + GLYOOA : 2.00E-18*0.5 ;
//2. KDEC C5DICARB + O3 = MGLYOX + .125 HCHO + .18 GLYOO + 0.82 HO2 + .57 OH + 1.265 CO : 2.00E-18*0.5 ;
//3. All merged C5DICARB + O3 = .5 GLYOX + .063 CH3CHO + .348 CH3CO3 + .285 CO + .285 OH + .063 HO2 +.09 MGLOO + .5 MGLYOX + .063 HCHO + .09 GLYOO + 0.41 HO2 + .285 OH + .633 CO
Aro157: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2
Aro159: updated `rco3_o3`
Aro160: updated `rco3_ooh`
Aro161: updated `rco3_oh`
Aro165: Only major channel taken
Aro167: KDEC TLFUONOOA →.5 CO + .5 OH + .5 MECOACETO2 + .5 TLFUONOO and H2Osubs TLFUONOO →.625 C24O3CCO2H + .375 ACCOMECHO + .375 H2O2

Aro169: updated `rco3_ooh`+`rco3_o3`
Aro170: updated `rco3_oh`

Aro180: KDEC C4M2ALOHO → GLYOX + MGLYOX + HO2
Aro181: KDEC C4M2ALOHO → GLYOX + MGLYOX + HO2
Aro182: Only major channel taken
Aro193: KDEC C4M2ALOHO2 →GLYOX + MGLYOX + HO2
Aro194: updated `rco3_oh` and KDEC C3MCODBCO2 → .35 MGLYOX + .35 HO2 + .35 CO + .65 MMALANHY + .65 HO2
Aro195: updated `rco3_ooh`+`rco3_o3`
Aro196: KDEC C3MCODBCO2 → .35 MGLYOX + .35 HO2 + .35 CO + .65 MMALANHY + .65 HO2
Aro198: KDEC C3MCODBCO2 → .35 MGLYOX + .35 HO2 + .35 CO + .65 MMALANHY + .65 HO2
Aro199: KDEC C3MCODBCO2 → .35 MGLYOX + .35 HO2 + .35 CO + .65 MMALANHY + .65 HO2

Aro205: KDEC NTLFUO → ACCOMECHO + NO2
Aro206: KDEC NTLFUO → ACCOMECHO + NO2
Aro207: KDEC NTLFUO → ACCOMECHO + NO2

Aro218: KDEC C5DIALO →MALDIAL
Aro219: KDEC C5DIALO →MALDIAL
Aro220: KDEC C5DIALO →MALDIAL

Aro227: KDEC C615CO2O → C5DICARB + CO + HO2
Aro228: KDEC C615CO2O → C5DICARB + CO + HO2
Aro229: Only major channel taken

Aro237: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2
Aro238: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2
Aro239: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2
Aro241: KDEC CATECOOA → MALDALCO2H + HCOCO2H + HO2 + OH
Aro247: updated `rco3_ooh`+`rco3_o3`
Aro248: updated `rco3_oh`
Aro254: KDEC GLYOOA → .125 HCHO + .18 GLYOO + .82 HO2 + .57 OH + 1.265 CO

Aro258: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2
Aro259: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2
Aro260: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

Aro264: KDEC NPHENO → MALDALCO2H + GLYOX + NO2
Aro265: KDEC NPHENO → MALDALCO2H + GLYOX + NO2
Aro266: KDEC NPHENO → MALDALCO2H + GLYOX + NO2
Aro267: merged equations

Aro275: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2
Aro276: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2
Aro277: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2
Aro284: merged equations(same rate c.)
Aro285: merged equation(same rate c.)

Aro290: KDEC PHENO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2
Aro291: KDEC PHENO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2
Aro292: KDEC PHENO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2 and Only major channel taken
Aro294: updated `rco3_ooh`+`rco3_o3`
Aro295: `rco3_oh`

Aro306: HOC6H4NO2 is a nitro-phenol

Aro312: KDEC PBZQO →C5CO2OHCO3
Aro313: KDEC PBZQO →C5CO2OHCO3
Aro314: KDEC PBZQO →C5CO2OHCO3 and Only major channel taken

Aro318: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2
Aro319: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2
Aro320: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

Aro325: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO
Aro326: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO
Aro327: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO and Only major channel taken

Aro335: KDEC NBZQO → C6CO4DB + NO2
Aro336: KDEC NBZQO → C6CO4DB + NO2
Aro337: KDEC NBZQO → C6CO4DB + NO2

Aro347: updated `rco3_o3`
Aro348: updated `rco3_ooh`
Aro349: updated `rco3_oh`
Aro353: Only major channel taken

Aro361: merged eq. under same rate c.

Aro365: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

Aro366: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE and Only major channel taken

Aro368: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2

Aro370: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2

Aro371: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2 and C6H5CH2OH replaced with its ox. product BENZAL

Aro372: merged eq under the same rate C.

Aro373: merged eq under the same rate C.

Aro375: KDEC TLBIPERO →.6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

Aro377: KDEC TLBIPERO →.6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DB COD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

Aro378: Only major channel and KDEC TLBIPERO →.6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DB COD + .2 C5DICARB + .2 TLFUONE + .2 BZ-FUONE + .2 MALDIAL

Aro380: KDEC MGLOOB → .125 CH3CHO + .695 CH3CO3 + .57 CO + .57 OH + .125 HO2 +.18 MGLOO

Aro381: merged equations

Aro388: KDEC CRESO → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

Aro389: KDEC CRESO → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

Aro390: KDEC CRESO → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE and Only major channel taken

Aro393: KDEC NCRESO → C5CO14OH + GLYOX + NO2

Aro394: KDEC NCRESO → C5CO14OH + GLYOX + NO2

Aro395: KDEC NCRESO → C5CO14OH + GLYOX + NO2 and Only major channel taken

Aro396: TOL1OHNO2 is a nitro-phenol

Aro399: KDEC MCATECOOA → MC3ODBCO2H + HCOCO2H + HO2 + OH

Aro404: updated `rco3_oh`

Aro405: updated `rco3_o3`

Aro406: updated `rco3_ooh`

Aro410: Only major channel taken

Aro415: KDEC TLEMUCO→ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

Aro416: KDEC TLEMUCO→ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2 and Only major channel taken

Aro417: branching ratios from Roth et al 2010

Aro418: branching ratios from Roth et al 2010

Aro419: branching ratios from Roth et al 2010

Aro465: KDEC NPTLQO → C7CO4DB + NO2

Aro466: KDEC NPTLQO → C7CO4DB + NO2

Aro467: KDEC NPTLQO → C7CO4DB + NO2

Aro470: KDEC PTLQO → C6CO2OHCO3

Aro471: KDEC PTLQO → C6CO2OHCO3

Aro472: Only major channel taken and KDEC PTLQO → C6CO2OHCO3

Aro482: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

Aro483: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

Aro487: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

Aro488: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

Aro489: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

Aro493: RO2 with ether function.

Aro495: KDEC MCOCOMOXO → HCHO + CH3CO3

Aro496: KDEC MCOCOMOXO → HCHO + CH3CO3

Aro497: KDEC MCOCOMOXO → HCHO + CH3CO3

Aro503: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

Aro504: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

Aro505: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

Aro508: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

Aro509: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

Aro510: KDEC DNCRESO → NC4MDCO2H +

HCOCO2H + NO2
Aro517: updated `rco3_oh`
Aro518: updated `rco3_ooh`+`rco3_o3`
Aro528: For consistency, we use the same products as for TOLUENE
Aro529: For consistency, we use the same products as for TOLUENE
Aro530: For consistency, we use the same products as for TOLUENE
Aro531: For consistency, we use the same products as for TOLUENE
Aro532: For consistency, we use the same products as for TOLUENE
Aro533: For consistency, we use the same products as for TOLUENE
Aro534: For consistency, we use the same products as for TOLUENE
Aro535: For consistency, we use the same products as for TOLUENE
Aro536: For consistency, we use the same products as for TOLUENE
Aro537: For consistency, we use the same products as for TOLUENE
Aro538: merged under same rate constant
Aro539: For consistency, we use the same products as for TOLUENE
Aro540: we use DIET35TOL(from MCM) as representative of Higher aromatics
Aro541: For consistency, we use the same products as for TOLUENE
Aro543: KDEC CH2OOB → .24 CH2OO + .40 CO + .36 HO2 + .36 CO + .36 OH and H2Osubs PHCHOO → .625 PHCOOH + .375 BENZAL + .375 H2O2
Aro546: KDEC NSTYRENEO → NO2 + HCHO + BENZAL
Aro547: KDEC NSTYRENEO → NO2 + HCHO + BENZAL
Aro548: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

Aro552: KDEC STYRENO → HO2 + HCHO + BENZAL
Aro553: KDEC STYRENO → HO2 + HCHO + BENZAL
Aro554: KDEC STYRENO → HO2 + HCHO + BENZAL

- 1) Several rate constant have been defined at the beginning of the gas.eqn file for practical reasons (but rate constants themselves have not been modified)
```
KRO2AP      = 1.00E-11
KRO2sHORO2 = 1.40E-12
KRO2tHORO2 = 1.60E-13
KRO2pRO2   = 1.30E-12
KRO2sRO2   = 2.50E-13
KRO2tRO2   = 6.70E-15
KRO2pORO2  = 2.00E-12
KRO2sORO2  = 8.80E-12
KRO2tORO2  = 9.20E-14
KPHENO2NO2 = 7.00E-12
```
and `rchohch2o2_oh = 0.10` from **?** and Groß (2013)

  The following rate constants have been updated (respect to those used in MCM) Groß (2013)
```
rco3_oh   = 0.69
rco3_o3   = 0.10
rco3_ooh  = 0.21
```

- 2) Species which react fast are substituted with the respective products of the major loss pathway (see MIM2). This includes ROO + H2O reactions
- 3) Alcohol and the aldehyde channels are minor of an already minor channel for RO2. We remove them.
- 4) Channel of OH formation added in reactions with KRO2HO2
- 5) Alkyl nitrates rate constant have been modified to be temperature dependent
- 6) LXYL and LTMB Rate constant for lumped aromatics where estimated by averaging the rate constant for the different isomers.

—- END of Aromatic gas phase reactions notes ———

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

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined

as:

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

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

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

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

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

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
AroJ001	TrGCJ	MCOCOMOOOH + hν → $CH_3C(O)OO$ + HCHO + OH	J_ACETOL+jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ002	TrGCJ	C33CO + hν → CO + HO_2 + CO + CO + HO_2	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
AroJ003	TrGCJ	C3DIALOOH + hν → GLYOX + CO + HO_2 + OH	jx(ip_HOCH2CHO)*2+jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ004	TrGCJ	C5DIALCO + hν → MALDIALCO3 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ005	TrGCJ	C32OH13CO + hν → GLYOX + HO_2 + HO_2 + CO	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
AroJ006	TrGCJ	HCOCOHCO3H + hν → GLYOX + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ007	TrGCJ	MALDIALOOH + hν → C32OH13CO + CO + OH + HO_2	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
AroJ008	TrGCJ	MALDIALOOH + hν → GLYOX + GLYOX + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ009	TrGCJ	BZFUOOH + hν → CO14O3CHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ010	TrGCJ	HOCOC4DIAL + hν → HCOCOHCO3 + HO_2 + CO	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ011	TrGCJN	NBZFUOOH + hν → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ012	TrGCJ	MALDALCO3H + hν → $HCOCO_3H$ + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ013	TrGCJ	MALDALCO3H + hν → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ014	TrGCJ	EPXDLCO2H + hν → C3DIALO2 + HO_2	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ015	TrGCJ	MALDIAL + hν → .4 BZFUONE + .6 MALDIALCO3 + .6 HO_2	4.E3*jx(ip_MVK)*0.14	Rickard and Pascoe (2009)
AroJ016	TrGCJ	MALANHYOOH + hν → HCOCOHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ017	TrGCJ	EPXDLCO3H + hν → C3DIALO2 + OH	jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ018	TrGCJ	CO2C4DIAL + hν → CO + CO + HO_2 + HO_2 + CO + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
AroJ019	TrGCJ	CO23C3CHO + hν → $CH_3C(O)OO$ + CO + CO + HO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ020	TrGCJ	CO23C3CHO + hν → $CH_3C(O)OO$ + $HCOCO_3$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ021	TrGCJ	MALDALCO2H + hν → $HCOCO_2H$ + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ022	TrGCJ	EPXC4DIAL + hν → C3DIALO2 + CO + HO_2	2.77*jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
AroJ023	TrGCJ	CO14O3CHO + hν → HO_2 + CO + HCOCH2O2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ024	TrGCJ	C23O3CHO + hν → CO + HO_2 + $CH_3C(O)OO$	J_ACETOL	Rickard and Pascoe (2009)
AroJ025	TrGCJ	C54CO + hν → HO_2 + CO + CO + CO + $CH_3C(O)OO$	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
AroJ026	TrGCJ	C5134CO2OH + hν → CO23C3CHO + HO_2 + CO + HO_2	jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ027	TrGCJ	C5DIALOOH + hν → MALDIAL + CO + HO_2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)*
AroJ028	TrGCNJ	NPXYFUOOH + hν → C23O3CCHO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ029	TrGCJ	C23O3CCHO + hν → CO + MCOCOMOXO2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ030	TrGCJ	PXYFUOOH + hν → C23O3CCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ031	TrGCJ	C5CO14OH + hν → $CH_3C(O)OO$ + $HCOCO_2H$ + HO_2 + CO	jx(ip_MVK)	Rickard and Pascoe (2009)
AroJ032	TrGCJ	C5DICARB + hν → .6 C5CO14O2 + .6 HO_2 + .4 TLFUONE	jx(ip_NO2)*0.2	Rickard and Pascoe (2009)*
AroJ033	TrGCJ	MC3ODBCO2H + hν → CH3COCO2H + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ034	TrGCJ	C4CO2DCO3H + hν → HO_2 + CO + C33CO + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ035	TrGCJ	ACCOMECHO + hν → MECOACETO2 + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ036	TrGCJ	MMALNHYOOH + hν → CO2H3CO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ037	TrGCJ	C5DICAROOH + hν → MGLYOX + GLYOX + HO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)*
AroJ038	TrGCNJ	NTLFUOOH + hν → ACCOMECHO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ039	TrGCJ	MECOACEOOH + hν → $CH_3C(O)OO$ + HCHO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ040	TrGCJ	C4MALOHOOH + hν → GLYOX + MGLYOX + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ041	TrGCJ	C4MALOHOOH + hν → CO2H3CHO + HO_2 + CO + OH	2.77*jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
AroJ042	TrGCJ	C5CO14OOH + hν → .83 MALANHY + .83 CH_3O_2 + .17 MGLYOX + .17 HO_2 + .17 CO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ043	TrGCJ	C4CODBCO3H + hν → .35 MGLYOX + .35 HO_2 + .35 CO + .65 MMALANHY + .65 HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ044	TrGCJ	C4CODBCO3H + hν → $HCOCO_3H$ + HO_2 + CO + $CH_3C(O)OO$	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ045	TrGCJ	TLFUOOH + hν → ACCOMECHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ046	TrGCJ	C23O3CCO3H + hν → OH + MCOCOMOXO2	jx(ip_CH3OOH)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
AroJ047	TrGCJ	MC3ODBCO3H + hν → CH3COCO3H + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ048	TrGCJ	MC3ODBCO3H + hν → .35 GLYOX + .35 CH_3O_2 + .35 CO + .65 MMALANHY + .65 HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ049	TrGCJ	ACCOMECO3H + hν → MECOACETO2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ050	TrGCJ	PHENOOH + hν → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ051	TrGCJ	C6CO4DB + hν → C4CO2DBCO3 + HO_2 + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
AroJ052	TrGCJ	C5CO2DCO3H + hν → $CH_3C(O)OO$ + C33CO + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ053	TrGCNJ	NDNPHENOOH + hν → NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ054	TrGCNJ	BZBIPERNO3 + hν → GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + NO_2	J_IC3H7NO3	Rickard and Pascoe (2009)*
AroJ055	TrGCNJ	HOC6H4NO2 + hν → HONO + PHONOnitrop + CPENTDIENKETENE	jx(ip_HOC6H4NO2)	see note
AroJ056	TrGCJ	CPENTDIENKETENE + hν → CO_2 + CO + 2 HO_2 + MALDIAL	J_KETENE	see note
AroJ057	TrGCJ	C5COOHCO3H + hν → HOCOC4DIAL + HO_2 + CO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ058	TrGCJ	BZEPOXMUC + hν → .5 C5DIALO2 + 1.5 HO_2 + 1.5 CO + .5 MALDIAL	jx(ip_NO2)*0.1	Rickard and Pascoe (2009)
AroJ059	TrGCJN	NPHEN1OOH + hν → NPHEN1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ060	TrGCJ	BZEMUCCO + hν → HCOCOHCO3 + C3DIALO2	jx(ip_HOCH2CHO)*2+J_ACETOL	Rickard and Pascoe (2009)
AroJ061	TrGCJ	BZEMUCCO2H + hν → C5DIALO2 + HO_2	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ062	TrGCNJ	NNCATECOOH + hν → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ063	TrGCJ	C615CO2OOH + hν → C5DICARB + CO + HO_2 + OH	jx(ip_MVK)+jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ064	TrGCNJ	NPHENOOH + hν → MALDALCO2H + GLYOX + OH + NO_2	J_IC3H7NO3 + jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ065	TrGCNJ	NCATECOOH + hν → NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ066	TrGCJ	PBZQOOH + hν → C5CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ067	TrGCJ	BZOBIPEROH + hν → MALDIALCO3 + GLYOX + HO_2	J_ACETOL	Rickard and Pascoe (2009)
AroJ068	TrGCJ	BZBIPEROOH + hν → GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
AroJ069	TrGCNJ	NBZQOOH + hν → C6CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ070	TrGCJ	CATEC1OOH + hν → CATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ071	TrGCJ	C6125CO + hν → C5CO14O2 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_MVK)	Rickard and Pascoe (2009)
AroJ072	TrGCNJ	DNPHENOOH + hν → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ073	TrGCJ	BZEMUCCO3H + hν → C5DIALO2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ074	TrGCJ	C6H5OOH + hν → C6H5O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ075	TrGCJ	BZEMUCOOH + hν → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO) *2	Rickard and Pascoe (2009)*
AroJ076	TrGCJ	BZEMUCOH + hν → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + HO_2	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)*
AroJ077	TrGCJN	BZEMUCNO3 + hν → EPXC4DIAL + NO_2 + GLYOX + HO_2	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
AroJ078	TrGCJ	TLEPOXMUC + hν → .5 C615CO2O2 + HO_2 + CO + .5 EPXC4DIAL + .5 $CH_3C(O)OO$	jx(ip_NO2)*0.1	Rickard and Pascoe (2009)
AroJ079	TrGCJ	C6H5CH2OOH + hν → BENZAL + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ080	TrGCJ	C6H5CH2NO3 + hν → BENZAL + HO_2 + NO_2	0.59*J_IC3H7NO3	Rickard and Pascoe (2009)*
AroJ081	TrGCJ	BENZAL + hν → HO_2 + CO + C6H5O2	jx(ip_BENZAL)	Atkinson et al. (2012)
AroJ082	TrGCJ	TLBIPEROOH + hν → .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ083	TrGCJN	TLBIPERNO3 + hν → .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO_2	J_IC3H7NO3	Rickard and Pascoe (2009)*
AroJ084	TrGCJ	TLOBIPEROH + hν → C5CO14O2 + GLYOX + HO_2	J_ACETOL	Rickard and Pascoe (2009)
AroJ085	TrGCJ	CRESOOH + hν → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ086	TrGCNJ	NCRESOOH + hν → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH + NO_2	J_IC3H7NO3	Rickard and Pascoe (2009)*
AroJ087	TrGCNJ	NCRESOOH + hν → C5CO14OH + GLYOX + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ088	TrGCNJ	TOL1OHNO2 + hν → HONO + PHONOnitrop + MCPENTDIENKETENE	jx(ip_TOL1OHNO2)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
AroJ089	TrGCJ	C4MDIAL + hν → .3 C3MCODBCO3 + .3 HO_2 + .3 CO + .3 MC3CODBCO3 + .3 HO_2 + .3 CO + .4 PXYFUONE	4.E3*jx(ip_MVK)*0.2	Rickard and Pascoe (2009)
AroJ090	TrGCJ	TLEMUCCO2H + hν → C615CO2O2 + HO_2	jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ091	TrGCJ	TLEMUCCO3H + hν → C615CO2O2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)
AroJ092	TrGCJ	TLEMUCOOH + hν → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH	jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)*
AroJ093	TrGCNJ	TLEMUCNO3 + hν → EPXC4DIAL + NO_2 + $CH_3C(O)OO$ + CO + HO_2	2.77*jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)
AroJ094	TrGCJ	TLEMUCCO + hν → $CH_3C(O)OO$ + EPXC4DIAL + CO + HO_2	2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
AroJ095	TrGCJ	C6H5CO3H + hν → C6H5O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ096	TrGCJ	OXYL1OOH + hν → TOL1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ097	TrGCNJ	MNCATECH + hν → HONO + PHONOnitrop + MCPENTDIENKETENE	jx(ip_TOL1OHNO2)	see note
AroJ098	TrGCJ	MCPENTDIENKETENE + hν → CO_2 + CO + 2 HO_2 + C4MDIAL	J_KETENE	see note
AroJ099	TrGCNJ	DNCRES + hν → HONO + PHONOnitrop + MNCPENTDIENKETENE + LhvDNCRES + NO_2	jx(ip_TOL1OHNO2)	see note
AroJ100	TrGCNJ	MNCPENTDIENKETENE + hν → CO_2 + CO + 2 HO_2 + NC4MDCO2HN	J_KETENE	see note
AroJ101	TrGCNJ	DNPHEN + hν → HONO + MNCPENTDIENKETENE + NO_2	jx(ip_HOC6H4NO2)	see note
AroJ102	TrGCJ	MCATEC1OOH + hν → MCATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ103	TrGCNJ	NPTLQOOH + hν → C7CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ104	TrGCJ	PTLQOOH + hν → C6CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ105	TrGCNJ	NCRES1OOH + hν → NCRES1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ106	TrGCNJ	MNNCATCOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ107	TrGCNJ	MNCATECOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ108	TrGCJ	C7CO4DB + hν → C5CO2DBCO3 + HO_2 + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
AroJ109	TrGCNJ	NDNCRESOOH + hν → NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
AroJ110	TrGCNJ	DNCRESOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
AroJ111	TrGCJ	C6COOHCO3H + hν → C5134CO2OH + HO_2 + CO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
AroJ112	TrGCJ	STYRENOOH + hν → HO_2 + HCHO + BENZAL + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*

*Notes:

J-values are calculated with an external module and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:
J(11) → jx(ip_COH2)
J(12) → jx(ip_CHOH)
J(15) → jx(ip_HOCH2CHO)
J(18) → jx(ip_MACR)
J(22) → jx(ip_ACETOL)
J(23)+J(24) → jx(ip_MVK)
J(31)+J(32)+J(33) → jx(ip_GLYOX)
J(34) → jx(ip_MGLYOX)
J(41) → jx(ip_CH3OOH)
J(53) → J($iC_3H_7ONO_2$)
J(54) → J($iC_3H_7ONO_2$)
J(55) → J($iC_3H_7ONO_2$)
J(56)+J(57) → jx(ip_NOA)

AroJ001: KDEC MCOCOMOXO → HCHO + CH3CO3
AroJ003: KDEC C3DIALO → GLYOX + CO + HO2
AroJ008: KDEC MALDIALO → GLYOX + GLYOX + HO2
AroJ009: KDEC BZFUO → CO14O3CHO + HO2
AroJ011: KDEC NBZFUO → .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2
AroJ013: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO
AroJ016: KDEC MALANHYO → HCOCOHCO3
AroJ027: KDEC C5DIALO → MALDIAL + CO + HO2
AroJ028: KDEC NPXYFUO → C23O3CCHO + NO2
AroJ030: KDEC PXYFUO → C23O3CCHO + HO2
AroJ032: KDEC TLFUONE → .6 C5CO14O2 + .6 HO2 + .4 TLFUONE
AroJ036: KDEC MMALANHYO → CO2H3CO3
AroJ037: KDEC C5DICARBO → MGLYOX + GLYOX + HO2
AroJ038: KDEC NTLFUO → ACCOMECHO + NO2
AroJ039: KDEC MECOACETO → CH3CO3 + HCHO
AroJ042: KDEC C5CO14CO2 → .83 MALANHY + .83 CH3O2 + .17 MGLYOX + .17 HO2 + .17 CO
AroJ043: KDEC C3MCODBCO2 → .35 MGLYOX + .35 HO2 + .35 CO + .65 MMALANHY + .65 HO2
AroJ045: KDEC TLFUO → ACCOMECHO + HO2
AroJ048: KDEC MC3CODBCO2 → .35 GLYOX + .35 CH3O2 + .35 CO + .65 MMALANHY + .65 HO2
AroJ050: KDEC PHENO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2
AroJ053: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2
AroJ054: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE
AroJ062: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2
AroJ065: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2
AroJ066: KDEC PBZQO → C5CO2OHCO3
AroJ068: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE
AroJ069: KDEC NBZQO → C6CO4DB + NO2
AroJ072: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2
AroJ075: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO
AroJ076: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO
AroJ079: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2
AroJ080: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2
AroJ082: KDEC TLBIPERO → .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL
AroJ083: KDEC TLBIPERO → .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2

C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

AroJ085: KDEC CRESO → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

AroJ086: KDEC CRESO → .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

AroJ087: KDEC NCRESO → C5CO14OH + GLYOX + NO2

AroJ092: KDEC TLEMUCO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

AroJ101: new channel

AroJ103: KDEC NPTLQO → C7CO4DB + NO2

AroJ104: KDEC PTLQO → C6CO2OHCO3

AroJ106: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

AroJ107: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

AroJ109: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

AroJ110: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

AroJ112: KDEC STYRENO → HO2 + HCHO + BENZAL

Table 3: Box model simulation set up

Variable	Value
Time period	(1-10)th - August
Latitude	10° south
Temperature	301K
Pressure	101325. Pa
Relative humidity	70%
Flux of Benzene	6.666 $\times 10^{10}$ mlc cm^{-2} s^{-1}
Flux of Toluene	3.333 $\times 10^{11}$ mlc cm^{-2} s^{-1}
Flux of Phenol	6.666 $\times 10^{10}$ mlc cm^{-2} s^{-1}
Flux of NO	3.333 $\times 10^{11}$ mlc cm^{-2} s^{-1}
Flux of DMS	6.666 $\times 10^{10}$ mlc cm^{-2} s^{-1}
Flux of CH3CHO	6.666 $\times 10^{10}$ mlc cm^{-2} s^{-1}

Table 4: Henry's coefficients assigned to aromatic compounds used in the chemical mechanism

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
BENZENE	*1.8* 10^{-1}	4100	*Benzene*	*Sander (2015)*
TOLUENE	*1.5* 10^{-1}	4000	*Toluene*	*Sander (2015)*
BENZAL	*3.6* 10^{1}		*Benzaldehyde*	*Sander (2015)*
MALANHY	3.6 10^{1}	0		
TLFUONE	3.6 10^{1}	0	5-Methyl-2(5H)-furanone	
C6H5CH2NO3	3.6 10^{1}	0		
BZFUONE	3.6 10^{1}	0		
PXYFUONE	3.6 10^{1}	0	3-Methyl-2(5H)-furanone	
PHENOL	*2.9* 10^{3}	*6800*	*Phenol*	*Sander (2015)*
C6H5O	2.9 10^{3}	6800	Phenyloxidanyl	
C6H5OOH	2.9 10^{3}	6800	Phenyl hydroperoxide	
C6H5CH2OOH	2.9 10^{3}	6800	Benzyl hydroperoxide	
TOL1O	2.9 10^{3}	6800	(2-Methylphenyl)oxidanyl	
C6H5CH2OH	2.9 10^{3}	6800		
OXYL1OOH	2.9 10^{3}	6800		
BZBIPERNO3	2.9 10^{3}	6800		
CRESOL	2.9 10^{3}	6800	Cresol	
HOC6H4NO2	*7.0* 10^{1}	*4600*	*2-nitrophenol*	Sander (2015)
NPHEN1OOH	7.0 10^{1}	4600		
NPHEN1O	7.0 10^{1}	4600		
TOL1OHNO2	7.0 10^{1}	4600		
NCRES1O	7.0 10^{1}	4600		
NCRES1OOH	7.0 10^{1}	4600		
TLBIPERNO3	7.0 10^{1}	4600		
PBZN	7.0 10^{1}	4600	benzoyl nitro peroxide	
NSTYRENOOH	7.0 10^{1}	4600		
DNPHEN	*2.3* 10^{3}	*0*	*dinitro-o-cresol*	*Sander (2015)*
NDNPHENOOH	2.3 10^{3}	0		
NNCATECOOH	2.3 10^{3}	0		

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
DNPHENOOH	2.3 10^3	0		
MNNCATCOOH	2.3 10^3	0		
DNCRESOOH	2.3 10^3	0		
NDNCRESOOH	2.3 10^3	0		
DNCRES	2.3 10^3	0	2-Methyl-4,6-dinitrophenol	
PHCOOH	*2.4* 10^4	0	*Benzoic Acid*	*Sander (2015)*
PTLQCO	2.4 10^4	0		
C6H5CO3H	2.4 10^4	0	Perbenzoic acid	
NBZQOOH	2.4 10^4	0		
NPTLQOOH	2.4 10^4	0		
NBZFUOOH	2.4 10^4	0		
STYRENOOH	2.4 10^4	0		
CATECHOL	4.6 10^3	0	Catechol	Sander (2015)
PBZQCO	4.6 10^3	0		
NPHENOH	4.6 10^3	0		
CATEC1O	4.6 10^3	0		
NPHENOOH	4.6 10^3	0		
NCRESOOH	4.6 10^3	0		
NCATECHOL	4.6 10^3	0		
CATEC1OOH	4.6 10^3	0		
MNCATECH	4.6 10^3	0	3-Methyl-6-nitro-1,2-benzenediol	
MCATECHOL	4.6 10^3	0	3-Methylcatechol	
MCATEC1OOH	4.6 10^3	0		
NCRESOH	4.6 10^3	0		
GLYOX	3.6 10^5	0	Glyoxal	Sander (2015)
C5DIALOOH	3.6 10^5	0		
BZEPOXMUC	3.6 10^5	0		
MALDIAL	3.6 10^5	0	2-Butenedial	
CO14O3CHO	3.6 10^5	0		
CO23C3CHO	3.6 10^5	0		
C54CO	3.6 10^5	0	2,3,4-Trioxopentanal	

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
EPXC4DIAL	3.6 10^5	0		
MGLYOX	3.7 10^3	7500	Methyl glyoxal	Sander (2015)
C5CO2DBPAN	3.7 10^3	7500		
C7CO4DB	3.7 10^3	7500		
GLYPAN	3.7 10^3	7500		
METACETHO	3.7 10^3	7500		
C23O3CHO	3.7 10^3	7500		
C23O3CCHO	3.7 10^3	7500		
C5DICARB	3.7 10^3	7500		
ACCOMECHO	3.7 10^3	7500		
C4MDIAL	3.7 10^3	7500		
C6125CO	3.7 10^3	7500	2,5-Dioxo-3-hexenal	
PAN	2.8 10^0	6500	peroxyacetylnitrate	Sander (2015)
C5COO2NO2	2.8 10^0	6500		
MC3CODBPAN	2.8 10^0	6500		
EPXDLPAN	2.8 10^0	6500		
ACCOMEPAN	2.8 10^0	6500		
C3MCODBPAN	2.8 10^0	6500		
C23O3CPAN	2.8 10^0	6500		
BZEMUCPAN	2.8 10^0	6500		
TLEMUCPAN	2.8 10^0	6500		
MALDIALPAN	2.8 10^0	6500		
CH3O2NO2	2.8 10^0	6500	(Nitroperoxy)methane	
PHAN	3.9 10^4	8600		Sander (2015)
TLOBIPEROH	3.9 10^4	8600		
C4CO2DBPAN	3.9 10^4	8600		
HCOCOHPAN	3.9 10^4	8600		
NC4DCO2H	3.9 10^4	8600		
C4PAN6	3.9 10^4	8600		
C5CO2OHPAN	3.9 10^4	8600		
BZEMUCNO3	3.9 10^4	8600		

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
TLEMUCNO3	3.9 10^4	8600		
C6CO2OHPAN	3.9 10^4	8600		
CH3OOH	3.2 10^2	5300	methyl hydroperoxide	Sander (2015)
3-Hexanol	2.0 10^1			Sander (2015)
2,5-hexanediol	2.0 10^6			Sander (2015)
C4M2AL2OH	2.0 10^6			
C4MALOHOOH	2.0 10^6			
C6COOHCO3H	2.0 10^6			
TLEMUCOOH	2.0 10^6			
HCOCOHCO3H	2.0 10^6			
MALDIALOOH	2.0 10^6			
MMALNHY2OH	2.0 10^6			
PHENOH	2.0 10^6			
MNCATECOOH	2.0 10^6			
BZFUOOH	2.0 10^6			
MALNHYOHCO	2.0 10^6			
MALANHYOOH	2.0 10^6			
MALANHY2OH	2.0 10^6			
BZFUOH	2.0 10^6			
PXYFUOOH	2.0 10^6			
TLFUOH	2.0 10^6			
MMALNHYOOH	2.0 10^6			
PXYFUOH	2.0 10^6			
TLFUOOH	2.0 10^6			
PHENOOH	2.0 10^6			
NCATECOOH	2.0 10^6			
PBZQOOH	2.0 10^6			
BZBIPEROOH	2.0 10^6			
BZBIPER2OH	2.0 10^6			
PBZQOH	2.0 10^6			
PTLQOH	2.0 10^6			

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
CRESOH	2.0 10^6			
TLBIPER2OH	2.0 10^6			
TLEMUCOH	2.0 10^6			
TLBIPEROOH	2.0 10^6			
MCATEC1O	2.0 10^6			
PTLQOOH	2.0 10^6			
CRESOOH	2.0 10^6			
HOHOC4DIAL	2.0 10^6			
CO2C4DIAL	2.0 10^6			
C514CO23OH	2.0 10^6			
C5DICAROOH	2.0 10^6			
C6CO4DB	2.0 10^6			
BZEMUCOOH	2.0 10^6			
BZEMUCOH	2.0 10^6			
C5COOHCO3H	2.0 10^6			
C4CO2DCO3H	2.0 10^6			
C5CO2DCO3H	2.0 10^6			
1,2,6-hexanetriol	2.0 10^{11}			Sander (2015)
trans-2-hexenal	2.0 10^1			Sander (2015)
MMALANHY	2.0 10^1			
PBZQONE	2.0 10^1		1,4-Benzoquinone	
NBZFUONE	2.0 10^1			
Glyoxylic acid	9.0 10^3			Sander (2015)
NC4MDCO2H	9.0 10^3			
BZEMUCCO2H	9.0 10^3			
BZEMUCCO	9.0 10^3			
BZEMUCCO3H	9.0 10^3			
BZFUCO	9.0 10^3			
MCOCOMOOOH	9.0 10^3			
CO14O3CO2H	9.0 10^3			
BZOBIPEROH	9.0 10^3			

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
NTLFUOOH	9.0 10^3			
C33CO	9.0 10^3		Oxomalonaldehyde	
C3DIALOOH	9.0 10^3			
C5DIALCO	9.0 10^3			
C32OH13CO	9.0 10^3			
MALDALCO3H	9.0 10^3			
EPXDLCO3H	9.0 10^3			
C615CO2OH	9.0 10^3			
EPXDLCO2H	9.0 10^3			
MALDALCO2H	9.0 10^3		4-Oxo-2-butenoic acid	
C5DIALOH	9.0 10^3			Sander (2015)
MC3ODBCO3H	9.0 10^3			
CH3COCO2H	3.1 10^5	5100	Piruvic Acid	Sander (2015)
C5134CO2OH	3.1 10^5	5100		
C23O3CCO2H	3.1 10^5	5100		
C24O3CCO2H	3.1 10^5	5100		
MECOACEOOH	3.1 10^5	5100		
C5CO14OOH	3.1 10^5	5100		
C4CODBCO3H	3.1 10^5	5100		
C23O3CCO3H	3.1 10^5	5100		
ACCOMECO3H	3.1 10^5	5100		
C615CO2OOH	3.1 10^5	5100		
CH3COCO3H	3.1 10^5	5100		
HOCOC4DIAL	3.1 10^5	5100		
TLEMUCCO	3.1 10^5	5100		
pentanoic acid	2.2 10^3	6583		Sander (2015)
C5CO14OH	2.2 10^3	6583		
MC3ODBCO2H	2.2 10^3	6583		
TLEMUCCO2H	2.2 10^3	6583		
TLEMUCCO3H	2.2 10^3	6583		
NPXYFUOOH	2.2 10^3	6583		

Table 4: Henry's coefficients (... continued)

aromatic species	**H [M/atm]**	$\Delta_{soln}H/\mathbf{R}$ **[K]**	**specie**	**Reference**
MVK	4.1 10^{1}			Sander (2015)
TLEPOXMUC	4.1 10^{1}			
PTLQONE	4.1 10^{1}		2-Methyl-1,4-benzoquinone	
TLEMUCCO	4.1 10^{4}			Warneck (2005)
LXYL	1.7 10^{-1}		xylene (averaged)	
O	1.9 10^{-1}		o-xylene	Sander (2015)
M	1.6 10^{-1}		m-xylene	Sander (2015)
P	1.6 10^{-1}		p-xylene	Sander (2015)
LTMB	2.2 10^{-1}		trimethylbenzene (ave)	
1,2,3	3.1 10^{-1}		1,2,3-trimethylbenzene	Sander (2015)
1,2,4	1.7 10^{-1}		1,2,4-trimethylbenzene	Sander (2015)
1,3,5	1.7 10^{-1}		1,2,5-trimethylbenzene	Sander (2015)
EBENZ	1.2 10^{-1}		ethylbenzene	Sander (2015)
HAROM	1.2 10^{-1}		3,5-dimethyl ethyl benzene	Sander (2015)
STYRENE	3.7 10^{-1}			Sander (2015)

The henry's coefficient is expressed as H (M/atm). The value that are assigned are taken from the compilation of Henry's coefficients by Rolf Sander unless specified otherwise. Many species are managed choosing surrogate species. Those species that have H $> 10^8$ need to be treated in SCAV as if they had H $= 10^8$ in order to avoid too high numerical stiffness.

The first row of each box is written in italics. This row is the reference structure value and chemical structure in which we have based our approximation for other species.

The criteria for choosing the Henry's coefficient for those species which is not defined is summarized in the following points:

1. Non-aromatic ring products: Hexanol (1OH), Hexanediol (2OH or OOH), Hexantril(3OH)
2. Conjugated carbonyls: Glyox (Doble aldehyde), Crotonaldehyde/trans-2-hexena (C5dicarb), 3-methyl butanoic acid (=O + -OH)
3. glyoxilic acid (aldehyde+carbonyl)

4. For species with more of 2-OH –¿10E6, which in the model is enough for an uptake of 90
5. -O- we consider it inert (epoxy group doesn't contribute efficiently. Epoxypropane Hr=5.3)
6. Not Hr for peroxy radicals (they react enough fast).They are not shown in the table.
7. We will tend to attach species to those of higher Rh (in case of doubt)

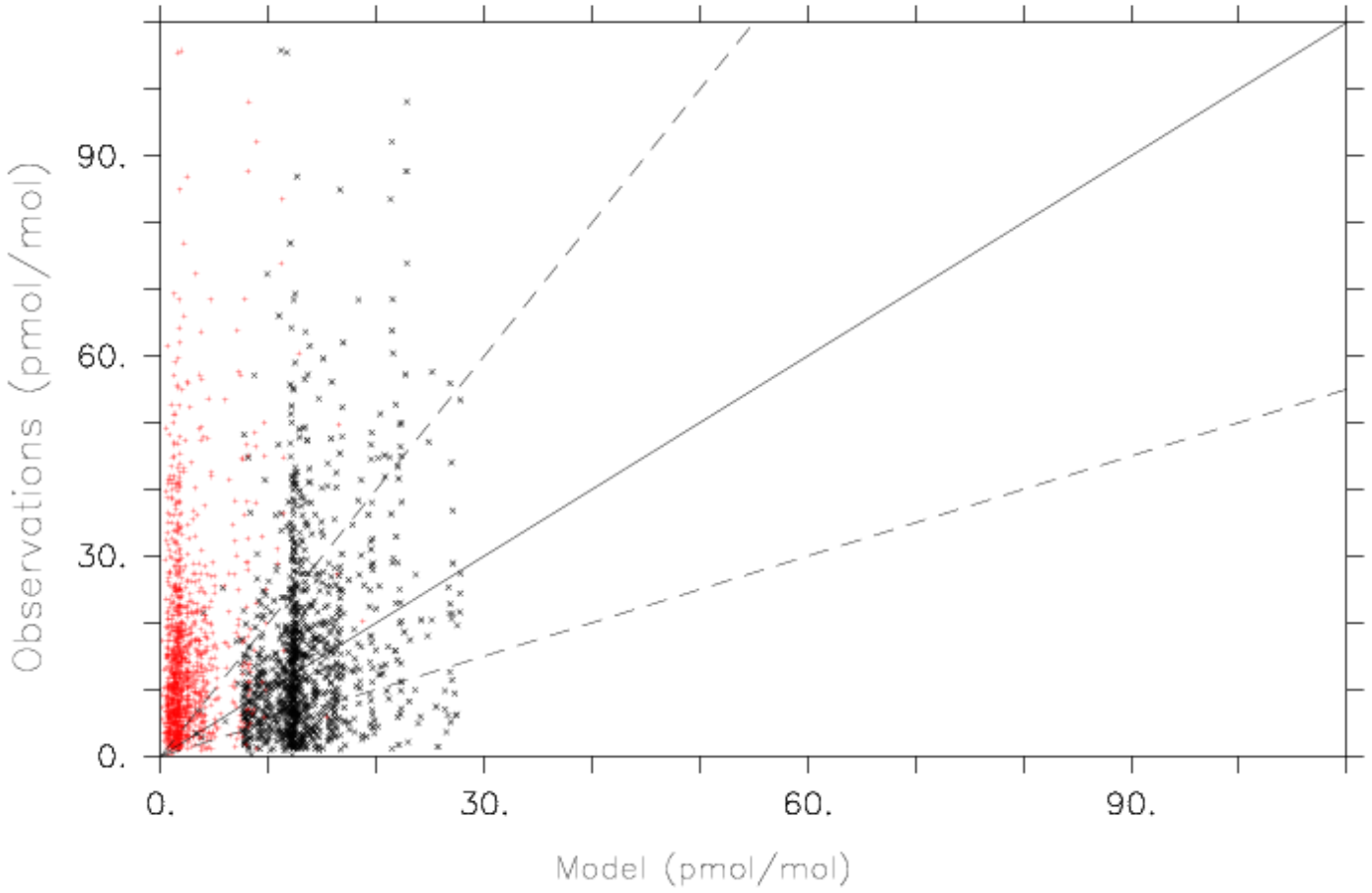

Figure 1: Scatter diagram of CARIBIC vs simulations (for benzene). In red LIT scenario, in black RCP scenario. Units are in pmol/mol

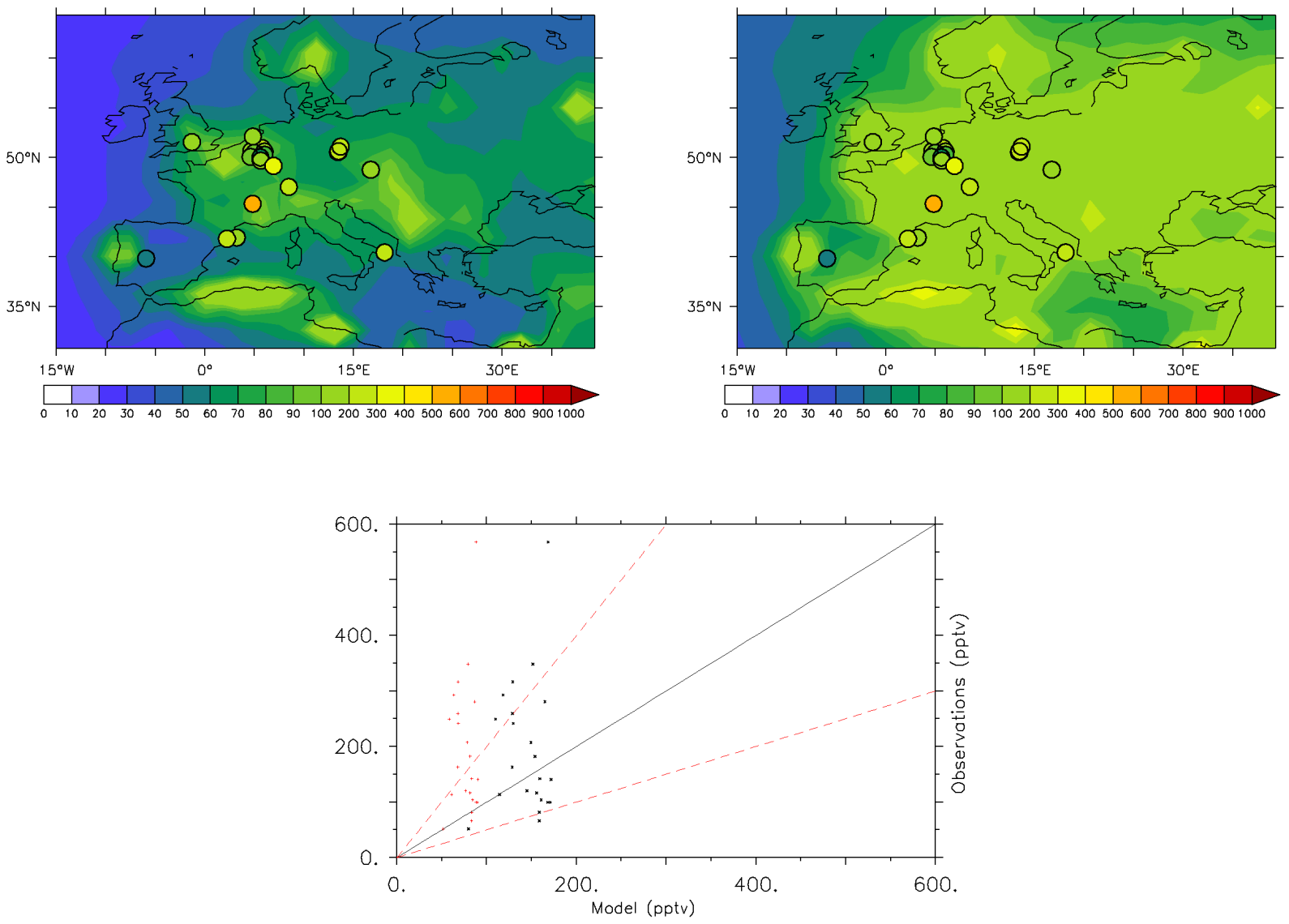

Figure 2: On top, benzene annual averaged mixing ratios for Europe (left LIT scenario, right RCP scenario). In circles, annual average mixing ratios of EEA dataset. Units are in pmol/mol. On the bottom, scatter plot of observations vs simulations. In red LIT scenario, in black RCP

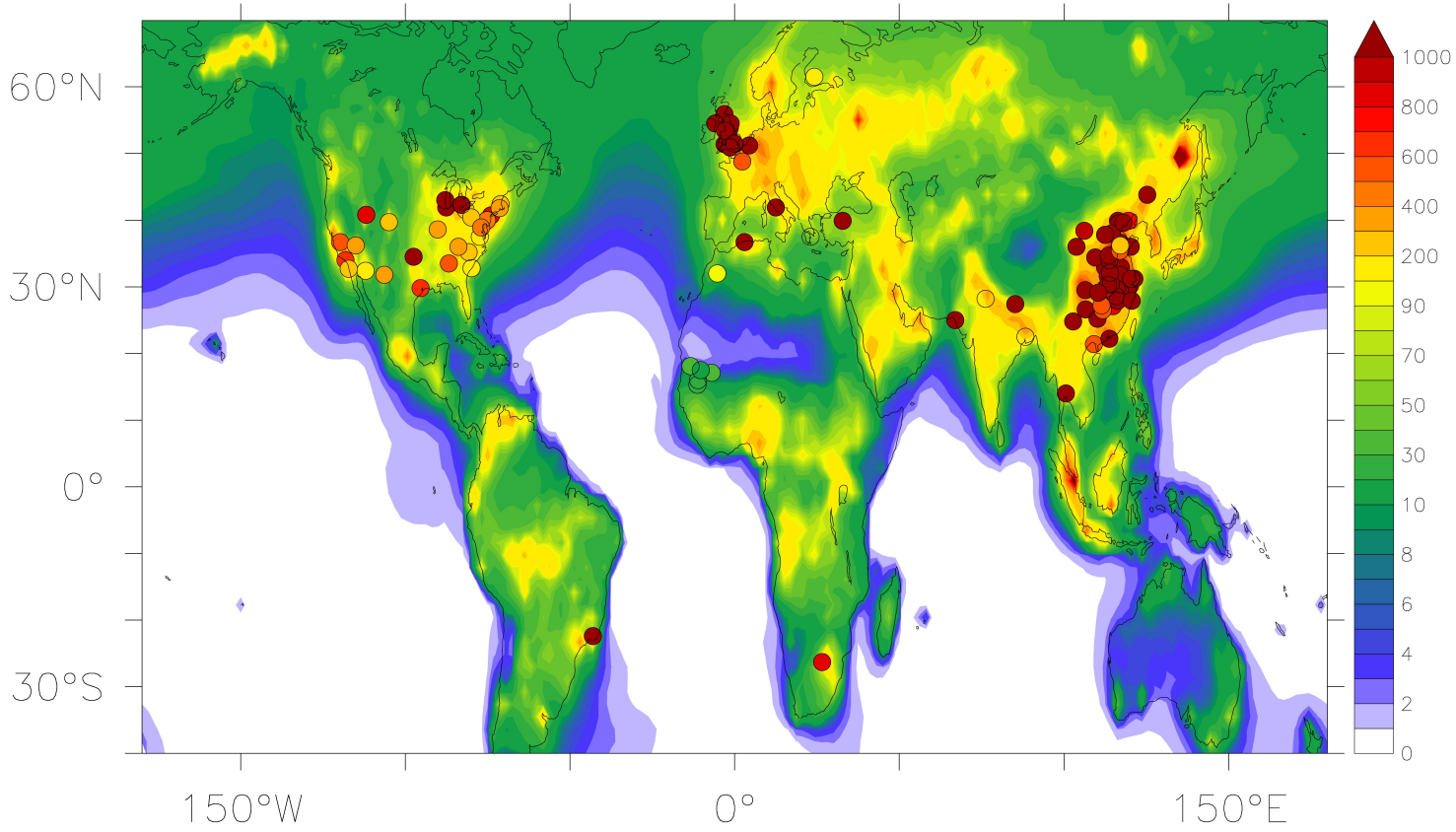

Figure 3: Toluene mixing ratios from literature in pmol/mol (each work covers different time spans). In background model annual average mixing ratios.

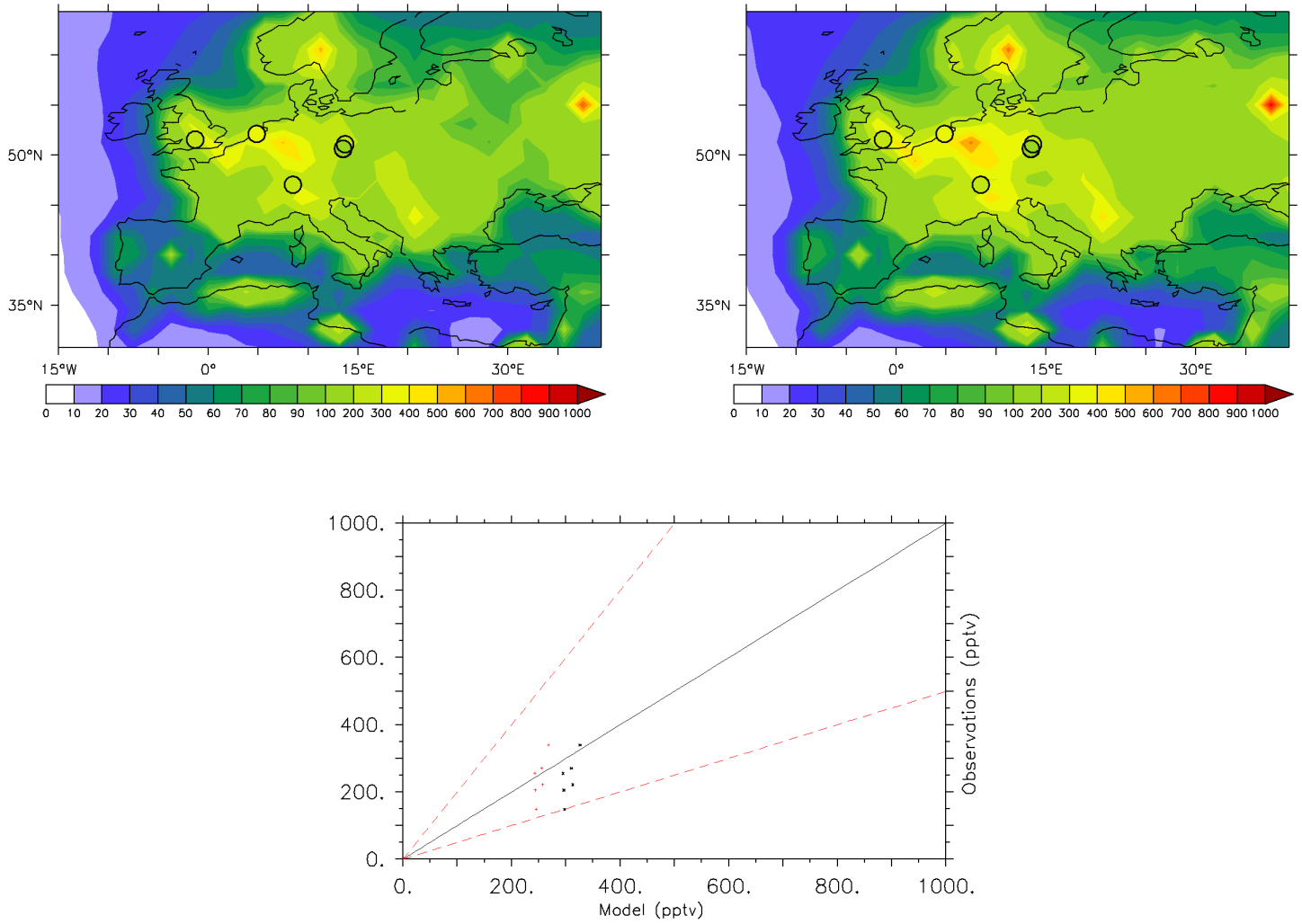

Figure 4: On top, toluene annual averaged mixing ratios for Europe (left LIT scenario, right RCP scenario). In circles, annual average mixing ratios of EEA. Units are in pmol/mol. On the bottom, scatter plot, in red LIT scenario, in black RCP

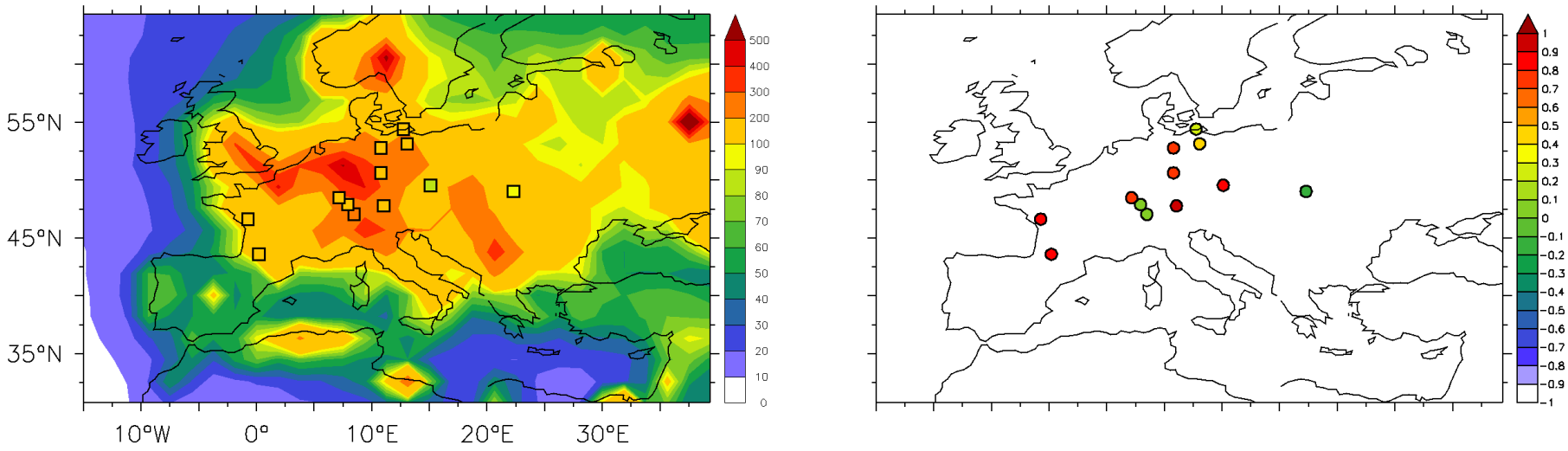

Figure 5: Left: In squares, toluene annual averaged mixing ratios of EMEP stations, in background LIT scenario annual averaged mixing ratios (in units of pmol/mol). Right: Temporal correlation between observations and simulated mixing ratios.

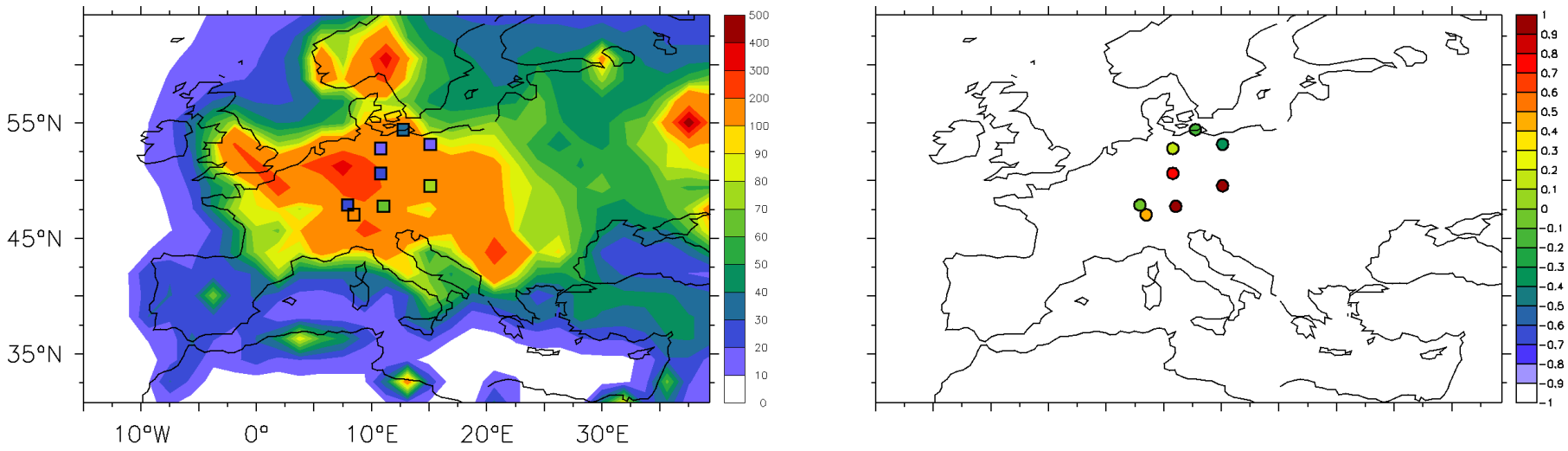

Figure 6: Left: In squares, xylene annual averaged mixing ratios of EMEP stations, in background LIT scenario annual averaged mixing ratios (in units of pmol/mol). Right: Temporal correlation between observations and simulated mixing ratios.

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