Supplementary information for

Gas-particle partitioning of toluene oxidation products: an experimental and modeling study

Victor Lannuque[1], Barbara D'Anna[2], Evangelia Kostenidou[2,a], Florian Couvidat[3], Alvaro Martinez-Valiente[2], Philipp Eichler[4,b], Armin Wisthaler[4,5], Markus Müller[6], Brice Temime-Roussel[2], Richard Valorso[7] and Karine Sartelet[1]

[1] CEREA, École des Ponts ParisTech, EDF R&D, IPSL, 77455 Marne-la-Vallée, France
[2] Aix-Marseille University, UMR 7673 CNRS, LCE, Marseille, France
[3] National Institute for Industrial Environment and Risks (INERIS), Verneuil-en-Halatte, France
[4] Institute for Ion and Applied Physics, University of Innsbruck, Innsbruck, 6020, Austria
[5] Department of Chemistry, University of Oslo, Oslo, 0315, Norway
[6] Ionicon Analytik GmbH, Innsbruck, 6020, Austria
[7] Univ Paris Est Creteil and Université de Paris, CNRS, LISA, 94010 Créteil, France
[a] Now at: Department of Environmental Engineering, Democritus University of Thrace, 67100 Xanthi, Greece
[b] Now at: German Environment Agency, Dessau, Germany

Correspondence to: Victor Lannuque (victor.lannuque@enpc.fr) and Barbara D'Anna (barbara.danna@univ-amu.fr)

Part 1: Instrumentation and experiments

Part 2: Modeling and chemical mechanisms

Part 1: Instrumentation and experiments

The PTR-ToF-MS drift tube was operated in the H_3O^+ mode with the same parameters for the gas phase and particle phase (CHARON) measurements: 2.35 mbar absolute pressure, 120°C temperature, and a reduced electric field strength of 105 Td (1 Td $=10^{-17}$ V cm^2). With the chosen instrumental parameters, ion hydration in the drift tube was still efficiently suppressed. Typical mass resolving power (FWHM) and mass accuracy values were 4000 and 13 ppm, respectively. A multicomponent calibration gas standard (Apel Riemer Environmental Inc., Miami, FL, USA) was used for characterizing the instrumental response to low molecular weight analytes (*m/z* <200). Typically, 99.5% of the signals in were below m/z 200. The instrumental background was determined by periodically diverting the sampling flow through a High-Efficiency Particulate Air filter (HC01-5N-B miniature HEPA capsule filter) placed upstream of the CHARON inlet. The CHARON enrichment factor was 25 for particles above 250 nm, 20 for particles of 200 nm and 8 for particles around 150 nm (Fig S1). Enrichment factors were determined using size selected ammonium nitrate particles as described by Eichler et al (2015).

PTR-MS ionization of organic analytes (with the exception of a few small hydrocarbons) occurs at the collisional rate, which can be accurately predicted by ion−molecule collision theories. (Ellis et al. 2013) We used the Langevin−Gioumousis−Stevenson theory (Langevin, 1903; Gioumousis and Stevenson 1958) instrumental response factors to pure hydrocarbons. The Su and Chesnavich parametrized capture rate theory (Su and Chesnavich, 1982) was used for calculating instrumental sensitivities of heteroatom-containing hydrocarbons. This means that instrumental response factor can be calculated from the molecular weight, isotropic molecular polarizability, and dipole moment of an analyte molecule. We used the observed m/z (−1 to account for the added proton) as a proxy for the molecular weight, assuming that analyte molecules do not fragment upon protonation. Isotropic molecular polarizabilities were determined from the analyte ions' elemental composition using the parametrization proposed by Bosque and Sales. (Bosque and Sales, 2002). Dipole moments cannot be predicted solely from the molecular sum formula, and a constant value of 2.75 D was used for all heteroatom-containing analyte ions. This value represents an average of typical dipole moments of oxygenated hydrocarbons (1−4.5 D). This introduces a maximum quantification uncertainty of ±40%. The major primary reaction product, methylglyoxal, has a very low dipole moment (μD = 0.992 D) and does not react with protonated water clusters $(H_2O)_nH+$ (n > 1). Ion chemistry kinetics is thus similar to benzene and benzene sensitivities were used for methylglyoxal quantification. Expected uncertainties are ± 20 % for methylglyoxal. Signals with unknown elemental composition were quantified using the acetone sensitivity as a proxy, the maximum uncertainty in the response factor being −30/+60%. The total mass concentration of SOA was calculated by summing the mass concentrations associated with all detected m/z peaks.

The HR-ToF-AMS data were analyzed using the standard software SQUIRREL v1.60E and PIKA v1.6C (Sueper, 2011) with Igor Pro 6.37 (Wavemetrics Inc.). A high efficiency particulate air (HEPA) filter installed in front of the instrument to sample ambient air for 15-30 minutes was used to evaluate the instruments detection limits calculated as three times the standard deviation of the measured chemical species. The ionization efficiency (IE) with respect to nitrate anions was calculated at the beginning and at the end of the campaign using nebulised 350 nm mobility diameter ammonium nitrate particles (BFSP software was used and values varied between $2.2 \times 10^{-7} – 2.5 \times 10^{-7}$). The relative IE (RIE) of ammonium was 3.7 based on the mass spectrum of ammonium nitrate data from IE calibrations. The RIE of sulfate was determined by comparing the theoretical and the measured concentration of a solution of ammonium nitrate and ammonium sulfate and was determined to be 1.3. For the organic fraction the default value of 1.4 was used. The AMS data were corrected by collection efficiency (CE) calculated by comparison to the SMPS volume using densities of 1.7 g/cm^3 for ammonium sulphate and 1.4 g/cm^3 for organics. The CE values varied from 0.35 for pure ammonium sulphate particles to 0.70 after SOA formation (above 8 µg/m^3). Size calibrations were conducted once using polyststyrene latex spheres (PSL). The instrument resolution varied from 1200-1400.

CHARON PTR-ToF-MS compound selection and interpretation

Saturation mass concentration log(C_i^*) values are here used to discriminate between parent and fragment ions (fig. S4). The procedure (Gkatzelis et al., 2018b) suggests that if the volatility of a specific ion $(M+H)^+$ is similar to that of the ion $(M+H\text{-}FG)^+$, where FG is a functional group, then this latter is considered a possible ion fragment. If the volatility of the ion $(M+H)^+$ is considerably lower than the one of $(M+H\text{-}FG)^+$ then this latter is considered a possible parent ion. Figure S4 in the supplementary document shows some of the $(M+H\text{-}H_2O)^+$ ions considered fragments (blue) close to the 1:1 line. While in red are shown $(M+H\text{-}H_2O)^+$ ions having higher volatility therefore considered as possible parent ions. The gray lines indicate the ±0.3 change in log(C_i^*). Error bars correspond to the error of the average (1σ).

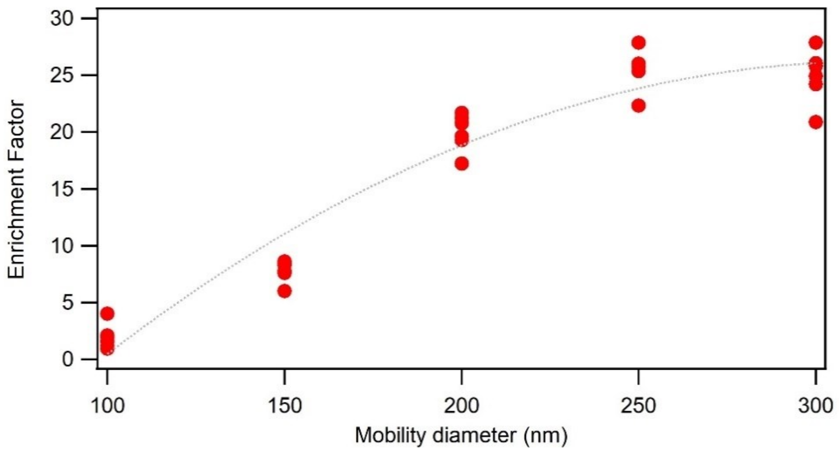


Figure S1: Enrichment factor calibration carried out with monodisperse particles of ammonium nitrate.

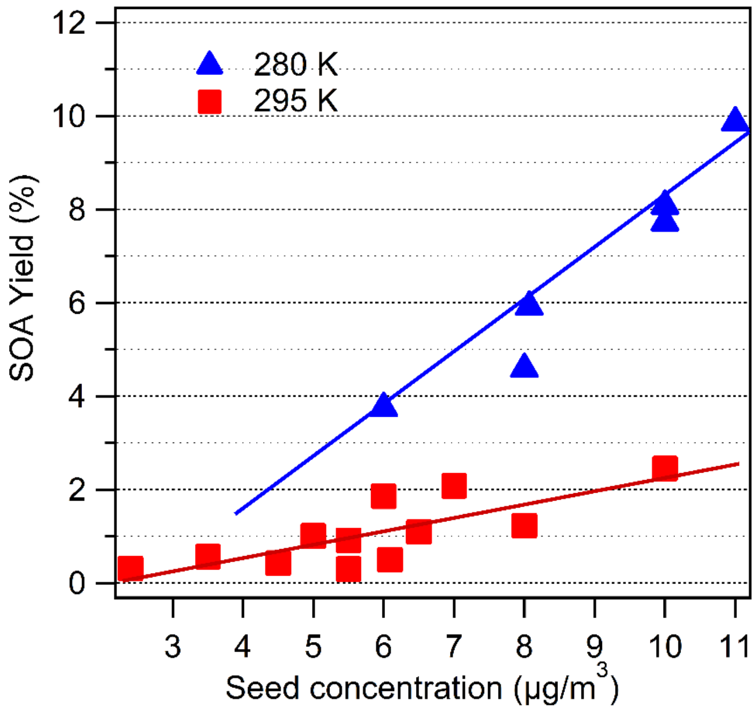


Figure S2: SOA yield derived as a function of seed concentration at 280K and 295K, respectively.

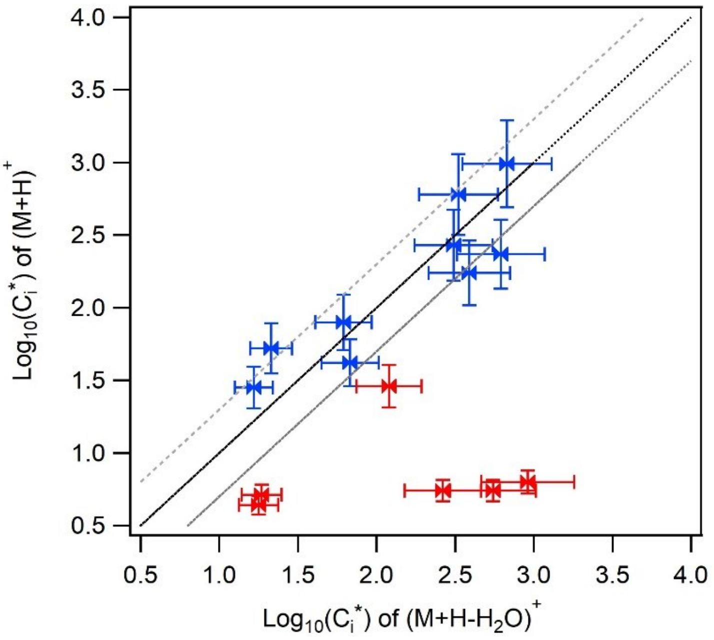


Figure S3: Fragment identification method from the toluene photo-oxidation experiments: correlation of the saturation concentration of identified $(M+H)^+$ ions to compounds with the same chemical formula subtracting water $(M+H-H_2O)^+$. For correlation close to the 1:1 line then the $(M+H-H_2O)^+$ compound is considered a fragment (blue). If the $(M+H-H_2O)^+$ ion shows a higher volatility, it is considered as a possible parent ion (red). The gray lines indicate the ±0.3 change in $log(C_i^*)$. Error bars correspond to the error of the average (1σ).

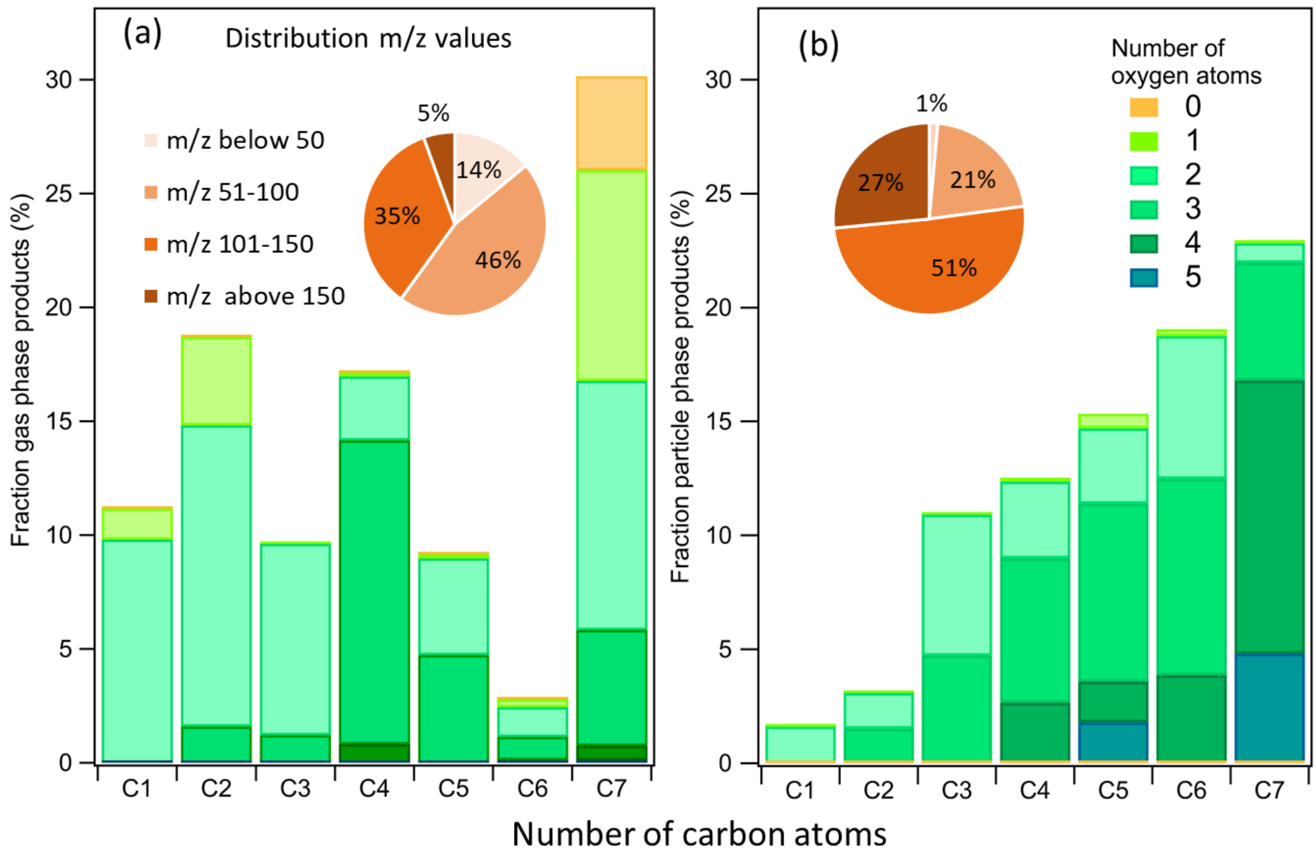


Figure S4: Mass products fraction (y-axis) distribution based on the number of carbon atoms (x-axis) for an experiment with 112 ppbv toluene at 295 K. Detected ions in the (a) gas phase and (b) particle phase. Pie charts correspond to the molecular weight contribution to the overall mass.

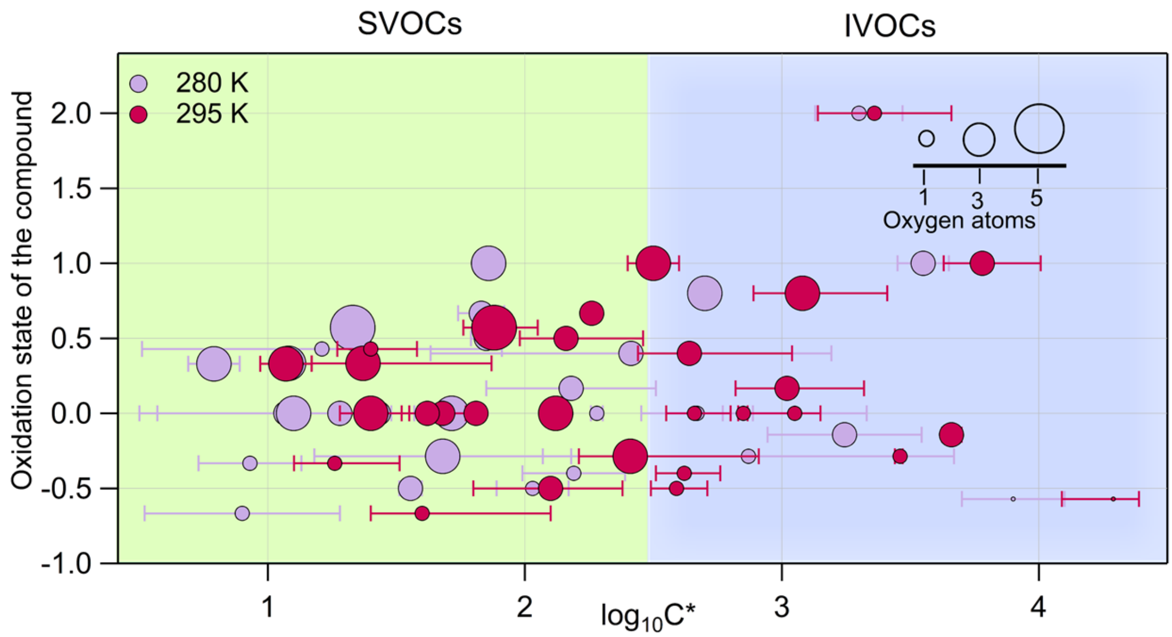


Figure S5: The oxidation state for the detected ions (OSc), versus the averaged saturation concentration in terms of $\log_{10}C_i^*$. The size of the dots denotes the oxygen atoms number. In light violet are represented the ions fragments identified for an experiment carried out at 280 K and in magenta those at 295 K. Errors bars correspond to ± 1σ of the experimental average.

Table S1: List of the experimental conditions, SOA concentration and yield.

No.	Temperature (K)	RH (%)	Intial Seed (μg/m^3)	Initial Toluene (ppbv)	OH conc. (10^7 cm^3)	SOA AMS (μg/m^3)	SOA Yield (%)
1	295	41	2.5	162	9.2	3.3	0.93
2	295	41	4.8	162	10.0	4.6	1.28
3	295	38	4.5	131	9.1	1.5	0.68
4	295	43	3.8	128	10.0	3.0	1.10
5	295	30	7.0	112	12.0	8.0	3.38
6	295	30	9.0	112	9.0	6.7	3.57
7	295	24	9.0	112	9.0	8.2	4.30
8	295	35	6.0	84	12.0	3.2	1.64
9	295	30	11.0	23	10.0	1.4	3.13
10	295	30	8.0	23	7.4	0.9	2.2
11	289	37	3.0	130	12.0	3.1	1.07
12	289	37	7.0	125	12.0	4.6	1.69
13	285	36	6.8	135	12.0	13.8	4.7
14	285	24	6.0	112	8.3	6.5	3.36
15	285	23	8.0	112	11.0	7.8	3.51
16	285	28	8.5	80	10.0	4.5	2.51
17	285	30	12.0	66	11.0	5.8	5.80
18	285	24	6.3	8	12.0	1.8	10.40
19	280	31	7.0	130	7.4	14.0	5.14
20	280	24	9.0	112	8.7	15.7	8.00
21	280	24	9.0	66	8.1	10.0	9.10
22	280	32	7.0	62	9.8	6.3	4.50
23	280	41	6.0	40	8.4	3.6	3.75
24	280	24	9.0	8	10.0	2.5	15.9

Table S2: Reference compounds ion distribution at 100 Td drift conditions, drift temperature 393 K and pressure 2.2 Torr. CHARON PTR-ToF-MS reference experiments were carried out by dissolving (when possible) the target reference compound in water then nebulized.

Compound	**Molecular formula**	**MW** (g/mol)	**PTR-MS** *m/z*	% Yield	**CHARON** *m/z*	% Yield
Formic acid	HCOOH	46.03	47.01	100	47.01	100
Methyl glyoxal	$C_3H_4O_2$	72.06	n.d.	n.d.	73.03 45.03	87 13
Butanal	C_4H_8O	72.11	73.06 55.05	16 84	n.d.	n.d.
Pentanal	$C_5H_{10}O$	86.13	87.08 69.06	14 86	n.d.	n.d.
Furaldehyde	$C_5H_4O_2$	96.08	97.03	100	n.d.	n.d.
Maleic Anhydride	$C_4H_3O_2$	98.06	99.01	100	99.01 117.02	95 5 (hydrate)
Benzaldehyde	C_7H_6O	106.12	107.05	100	n.d.	n.d.
Benzoquinone	$C_6H_4O_2$	108.09	109.03	100	109.03	100
Cresol	C_7H_8O	108.14	109.06	100	n.d.	n.d.
5-Methylfurfural	$C_6H_6O_2$	110.11	111.04	100	111.04	100
Succinic acid	$C_4H_6O_4$	118.09	n.d.	n.d.	119.03 101.02	2 98
5-Hydroxymethyl furfural	$C_6H_6O_3$	126.11	127.04 109.03	80 20	n.d.	n.d.
4-Nitrotoluene	$C_7H_7NO_2$	137.14	138.06	100	n.d.	n.d.
4-Nitrophenol	$C_6H_5NO_3$	139.11	140.04	100	140.04	100
4-Nitrocatechol	$C_6H_5NO_4$	155.11	156.03	100	156.03 125.03	91 9

Table S3: Derived logCi values and ion major identified parent and fragment ions.

Carbon number	Identified *m/z* and protonated molecular formula	Log Ci* at 295 K	Log Ci* at 280 K	∆Log Ci*
7	107.049 $(C_7H_6O)H^+$	4.28±0.08	3.09±0.11	0.37
7	123.046 $(C_7H_6O_2)H^+$	3.46±0.11	2.88±0.14	0.59
7	139.040 $(C_7H_6O_3)H^+$	2.19±0.07	1.75±0.11	0.47
7	141.054 $(C_7H_8O_3)H^+$	1.88±0.14	1.33±0.10	0.55
7	155.034 $(C_7H_6O_4)H+$	1.62±0.14	0.90±0.11	0.70
7	157.050 $(C_7H_8O_4)H$	1.37±0.50	1.08±0.17	0.29
7	171.029$(C_7H_6O_5)H+$	1.45±0.60	0.70±0.10	0.75
6	127.041 $(C_6H_6O_3)H^+$	1.46±0.25	0.83±0.05	0.63
6	143.034 $(C_6H_6O_4)$ H^+	1.26±0.03	0.93±0.02	0.33
6	125.029 $(C_6H_4O_2)$ H^+	1.40±0.30	1.10±0.30	0.30
6	129.057 $(C_6H_8O_3)H^+$	1.62±0.13	1.07±0.02	0.55
6	111.045 $(C_6H_6O_2)H^+$	2.10±0.03	1.56±0.05	0.55
6	140.039 $(C_6H_5NO_3)H+$	3.10±0.24	2.70±0.15	0.40
6	113.057$(C_6H_8O_2)H^+$	2.71±0.35	1.64±0.25	1.07
6	141.019 $(C_6H_4O_4)H^+$	1.75±0.13	1.38±0.03	0.37
6	95.050 $(C_6H_6O)H+$	2.60±0.20	2.08±0.05	0.52
6	109.030 $(C_6H_4O_2)H^+$	3.04±0.16	2.72±0.10	0.32
5	115.042 $(C_5H_6O_3)H^+$	1.81±0.34	1.43±0.02	0.39
5	101.060 $(C_5H_8O_2)H^+$	4.75±0.94	4.25±0.34	0.50
5	113.025 $(C_5H_4O_3)H^+$	2.69±0.36	2.41±0.14	0.28
5	99.046 $(C_5H_6O_2)H^+$	2.62±0.13	2.19±0.05	0.43
4	117.021 $(C_4H_4O_4)H^+$	2.50±0.60	1.89±0.05	0.65
4	103.042 $(C_4H_6O_3)H^+$	1.69±0.02	1.21±0.04	0.47
4	85.031 $(C_4H_4O_2)H^+$	2.66±0.12	2.29±0.05	0.38
4	87.046 $(C_4H_6O_2)H^+$	2.59±0.11	2.03±0.03	0.56
4	101.026 $(C_4H_4O_3)H^+$	2.35±0.24	1.87±0.04	0.48
4	83.014 $(C_4H_2O_2)H^+$	2.30±0.61	1.78±0.22	0.52
3	89.026 $(C_3H_4O_3)H^+$	2.24±0.11	1.83±0.02	0.42
3	71. 015$(C_3H_2O_2)H^+$	1.99±0.27	1.83±0.02	0.16
3	75.043 $(C_3H_6O_2)H^+$	4.40±0.52	2.55±0.19	0.85
3	73.030 $(C_3H_4O_2)H^+$	2.85±0.02	2.55±0.08	0.30
2	77.025 $(C_2H_4O_3)H+$	3.88±0.18	3.52±0.06	0.36
2	61.028 $(C_2H_4O_2)H^+$	3.76±0.49	3.04±0.06	0.72
1	47.013 $(CH_2O_2)H^+$	3.63±0.32	3.32±0.09	0.31

Part 2: Modeling and chemical mechanisms

Wall losses

A wall loss parameterization of gaseous organic compounds is implemented in SSH-aerosol for the modeling partitioning study of this work. In the absence of wall loss studies in Pyrex AFT, this parameterization follows the approach developed for Teflon chamber studies (Zhang et al., 2015; Huang et al., 2018; Krechmer et al., 2016). The parametrization represents an irreversible first-order process whose kinetics $k_{wall,i}$ (in s^{-1}) for the species i is calculated according to Eq. (S1):

$$k_{wall,i} = \left(\frac{A}{V}\right)\left(\frac{\pi}{2}\frac{1}{\sqrt{k_e D_g}} + \frac{4}{\alpha_{w,i}\,\bar{c_i}}\right)^{-1}, \tag{S1}$$

where A and V are the area (in m^2) and volume (in m^3) of the AFT, $\alpha_{w,i}$ and $\bar{c_i}$ are the wall accommodation coefficient and the mean molecular velocity (in m s^{-1}) of the species i and k_e and D_g are the eddy diffusivity coefficient (in s^{-1}) and the diffusivity in the gas phase (in m^2 s^{-1}). D_g is taken equal to 5×10^{-6} s^{-1}, k_e depends on the volume of the AFT and is calculated as:

$$k_e = 0.004 + 10^{-2.25}(V)^{0.74}, \tag{S2}$$

and $\bar{c_i}$ depends on the molar mass M_i (kg mol^{-1}) of species i:

$$\bar{c_i} = \sqrt{\frac{8RT}{\pi M_i}}, \tag{S3}$$

where R is the gas constant (R = 8,314 kg m^2 s^{-2} K^{-1} mol^{-1}), T is the temperature (in K). $\alpha_{w,i}$ depends on the saturation concentration C_i^* (in µg m^{-3}) of the species i according to the Eq. (S4) and Eq. (S5) do the link between C_i^* and P_i^{sat}:

$$\alpha_{w,i} = 10^a (C_i^*)^b, \tag{S4}$$

$$C_i^* = \frac{M_i \gamma_i P_i^{sat} \times 10^9}{RT}, \tag{S5}$$

with P_i^{sat} in Pa and where γ_i is the activity coefficient of the species i in the condensed phase (considered equal to 1 for this equation). a and b are tuning parameters. a is set to -2.744 as in Huang et al. (2018) for teflon chambers. b is here set to -1.407 so that the parameterization correctly reproduces the final SOA concentration of the studied case and allows the analysis of wall losses on the speciation and distribution of secondary organic compounds.

Irreversible partitioning of methylglyoxal

The oxidation of methylglyoxal in or at the surface of the aqueous phase can be considered as an irreversible gas-particle partitioning pathway as opposed to the reversible processes that are self-oligomerization and hydration (Hu et al., 2022). A simplified parametrization to represent the irreversible gas-particle partitioning of methylglyoxal depending on RH is also tested in the modeling partitioning study of this work. This empiric parameterization is based on effective uptake rates ($k_{eff,uptake}$) calculated with atmospheric observation values by Hu et al. (2022) for high RH cases (RH > 40%) and with experimental values by De Haan et al. (2018) for low RH cases (RH < 5%). A third-degree polynomial is fitted on experimental $k_{eff,uptake}$ to establish the RH dependency used in this study.

The empiric fit is here used to roughly estimate the $k_{eff,uptake}$ for the intermediate RH value of 24% of the simulated experiment. Polynomial and experimental $k_{eff,uptake}$ are presented in Fig. S7.

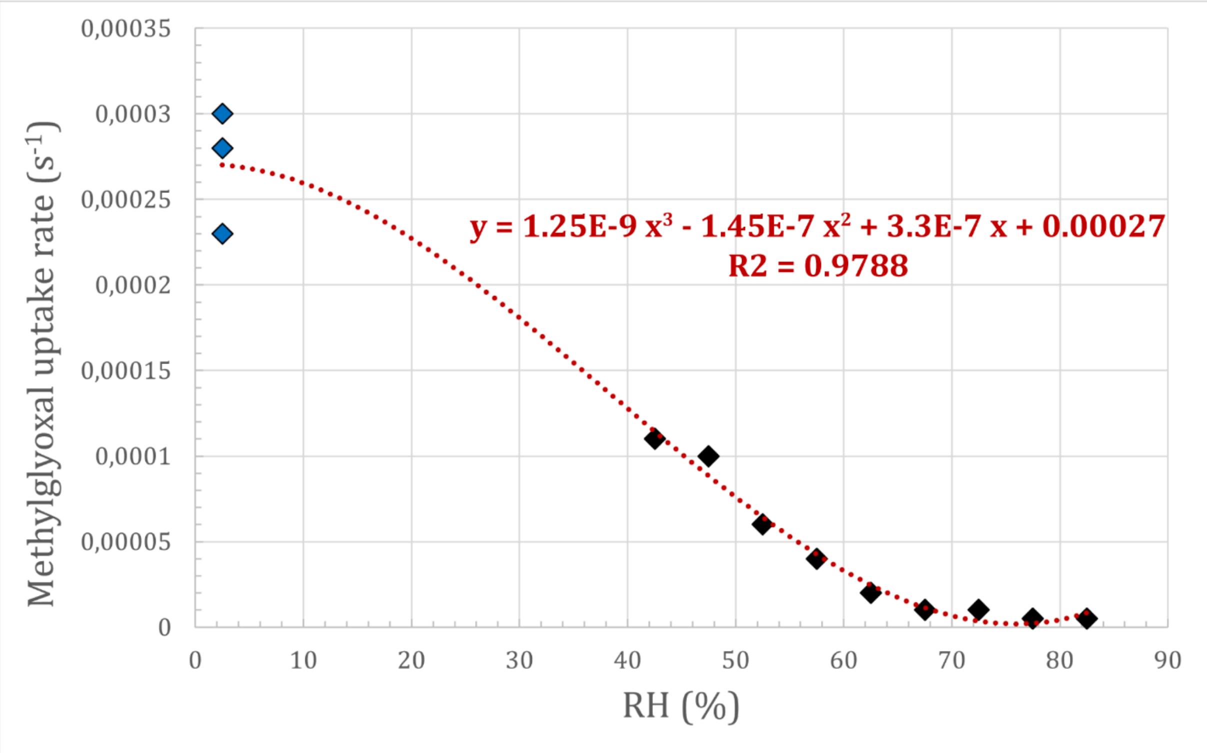


Figure S7: Experimental RH dependence of irreversible uptake rate of methylglyoxal. Blue points are from De Haan et al. (2018) and black points are from Hu et al. (2022).

Results and figures

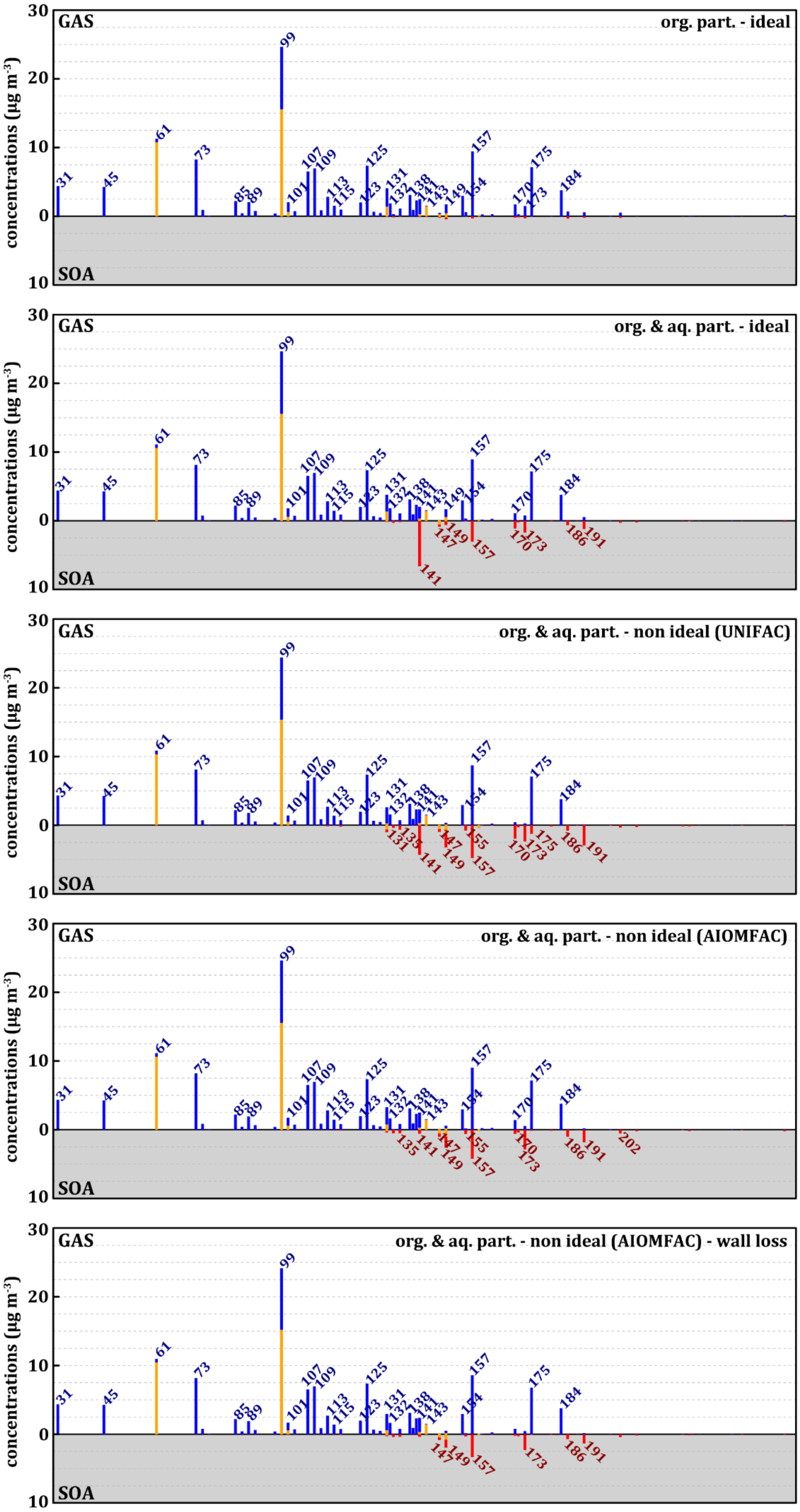


Figure S8: Mass spectra of gaseous (blue) and condensed (red) secondary compounds formed after 13 minutes of toluene oxidation under experimental conditions (see sect. 2.2.4) according to MG-

Cr-Al mechanism for the different partitioning tests. Yellow fraction of spectra represents recalculated mass after removing of functional groups with nitrogen for aliphatic compounds.

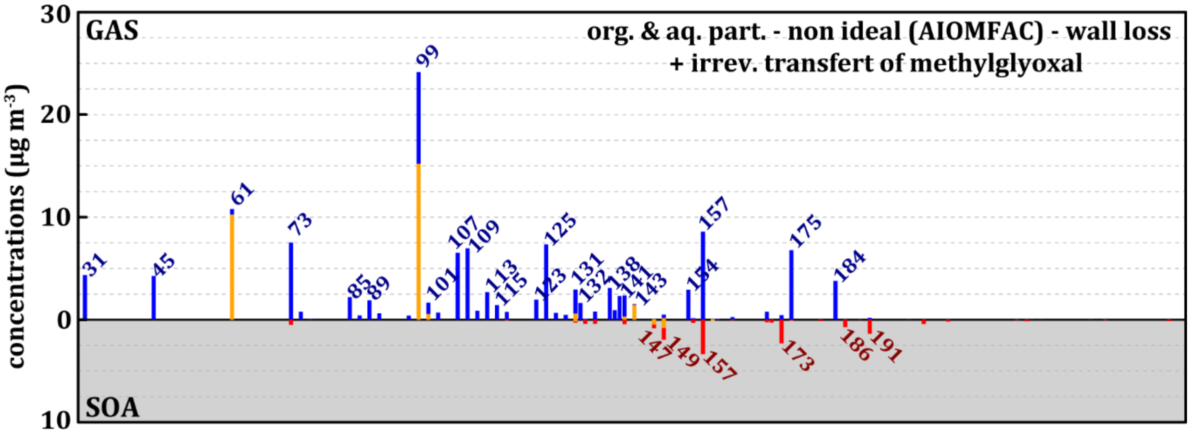


Figure S9: Mass spectra of gaseous (blue) and condensed (red) secondary compounds formed after 13 minutes of toluene oxidation under experimental conditions (see sect. 2.2.4) according to MG-Cr-Al mechanism considering partitioning both organic and aqueous phases with short-range interactions in both condensed phases and medium and long-range interactions in aqueous one only, wall losses of gaseous organic compounds and irreversible transfer to aqueous phase for methylglyoxal. Yellow fraction of spectra represents recalculated mass after removing of functional groups with nitrogen for aliphatic compounds.

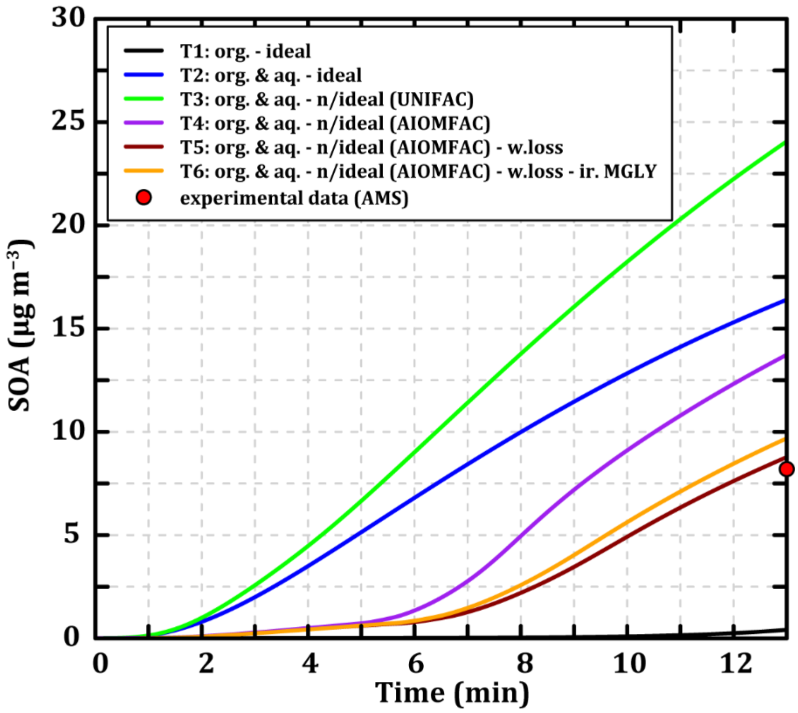
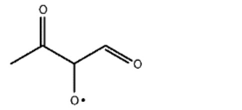
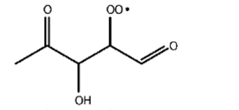
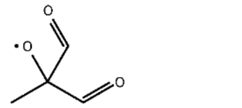
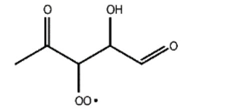
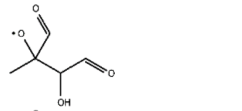
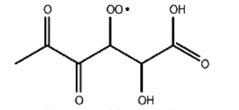
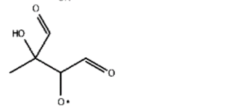
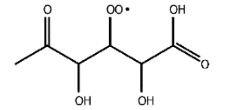
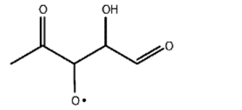
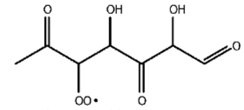
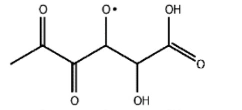
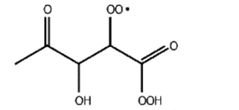
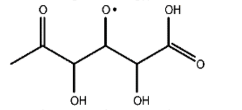
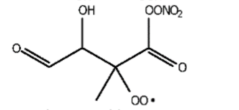
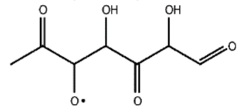
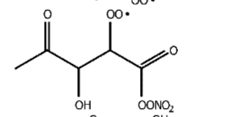
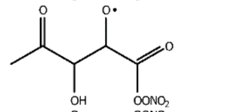
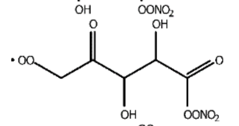
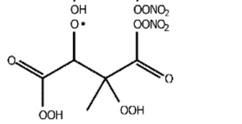
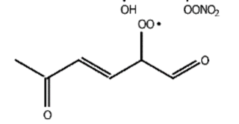
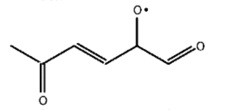
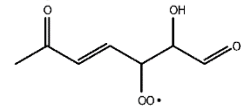
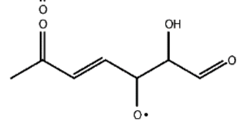
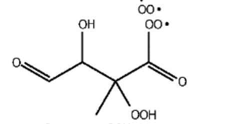
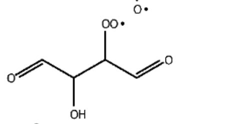
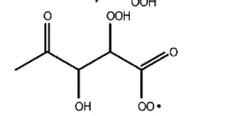
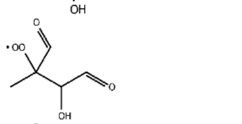
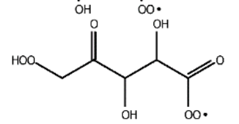
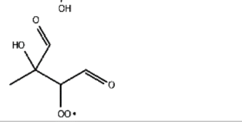
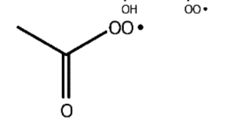


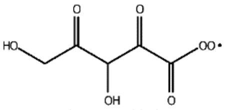
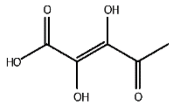
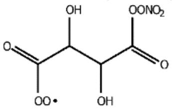
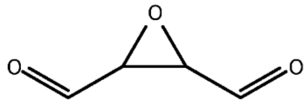
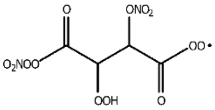
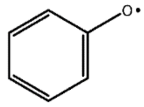
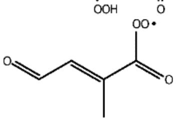
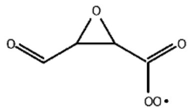
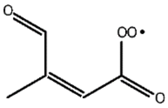
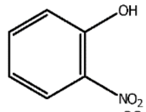
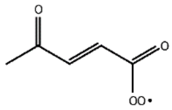
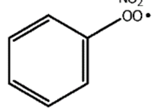
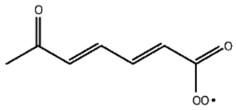
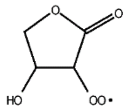
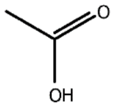
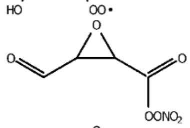
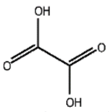
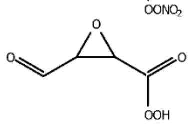
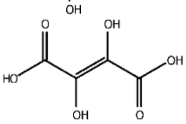
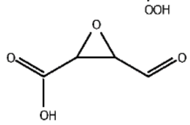
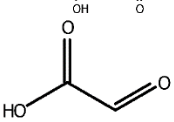
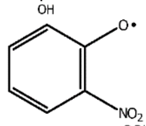
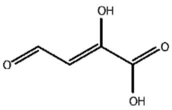
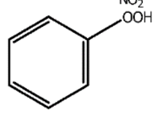
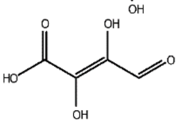
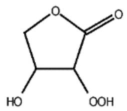
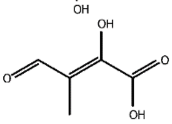
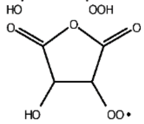
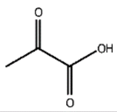
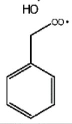
Figure S10: Temporal evolution of the SOA concentrations during toluene oxidation under experimental conditions (see sect. 2.2.3) simulated with MG-Cr-Al mechanism at 295 K considering mass transfer through an ideal organic phase (T1, black line), ideal organic and aqueous phases (T2, blue line), organic and aqueous phases with long-range interactions (T3, green line), organic and aqueous phases with long- and short-range interactions (T4, purple line), organic and aqueous phases with long- and short-range interactions and wall losses (T5, dark red

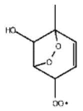
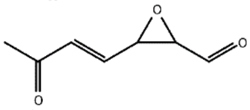
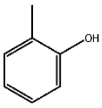
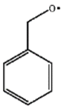
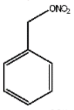
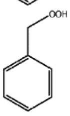
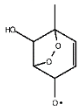
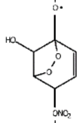
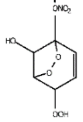
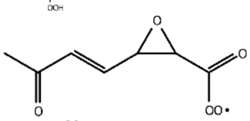
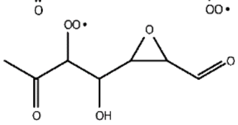
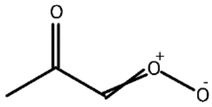
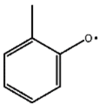
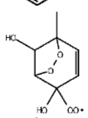
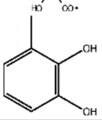
line) and organic and aqueous phases with long- and short-range interactions, wall losses and irreversible pathway for methylglyoxal condensation (T6, orange line). The red point represent the experimental SOA concentration measured by AMS.

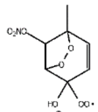
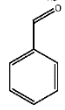
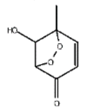
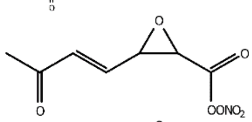
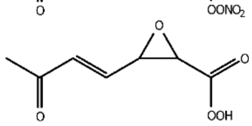
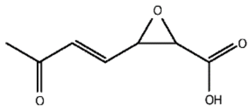
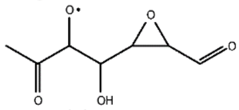
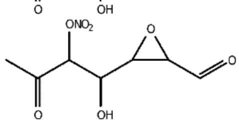
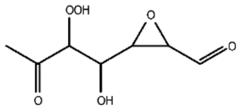
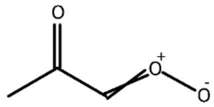
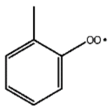
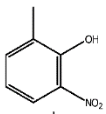
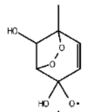
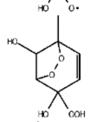
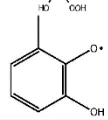
Chemical mechanisms

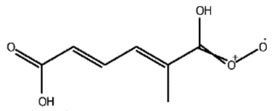
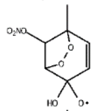
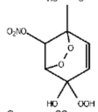
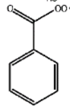
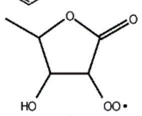
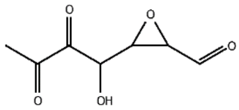
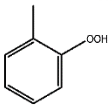
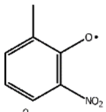
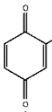
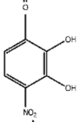
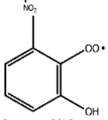
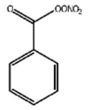
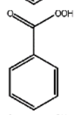
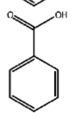
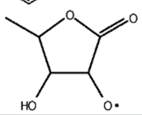
Table S4: Species list of MG-Cr-Al chemical mechanism.

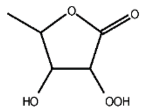
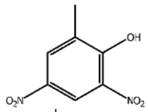
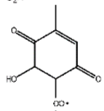
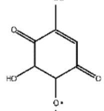
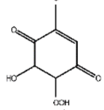
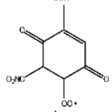
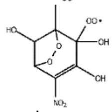
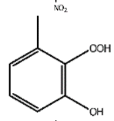
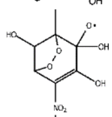
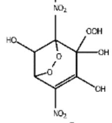
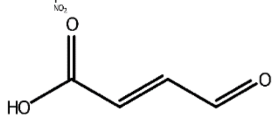
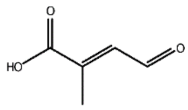
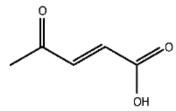
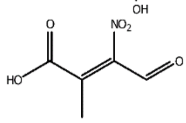
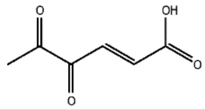
name	molecule (or position isomer)	name	molecule (or position isomer)
1D4000		2D5002	
1D4001		2D5003	
1D5000		2D6000	
1D5001		2D6001	
1D5003		2D7000	
1D6000		2G5006	
1D6001		2P5000	
1D7000		2P5006	
1P5006		2P500A	
1P500A		2U6000	
1U6000		2U7000	
1U7000		3H5000	
2D4000		3H5004	
2D5000		3H5009	
2D5001		3K2000	

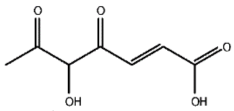
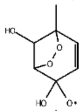
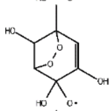
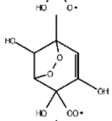
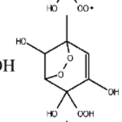
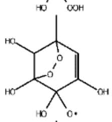
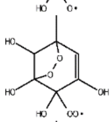
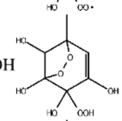
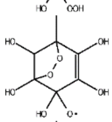
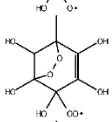
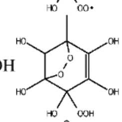
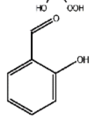
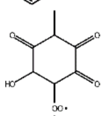
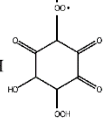
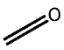
name	molecule (or position isomer)	name	molecule (or position isomer)
3K5003		AK5000	
3P4000		AR0010	
3P400X		AR0013	
3U5000		AR0020	
3U5001		AR0027	
3U5002		AR0028	
3U7000		AR0035	
A02000		AR0038	
AA2000		AR0039	
AA4000		AR0040	
AD2000		AR0042	
AD4000		AR0043	
AD4001		AR0048	
AD5000		AR0080	
AK3000		AR0085	

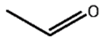
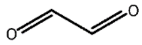
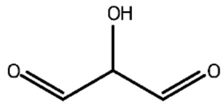
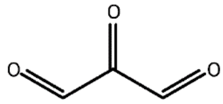
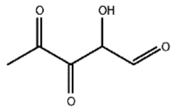
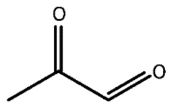
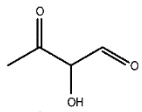
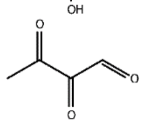
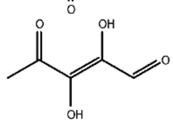
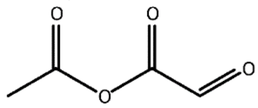
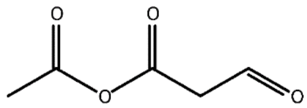
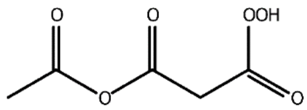
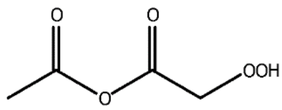
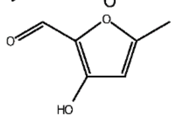
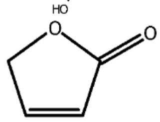
name	molecule (or position isomer)
AR0086	
AR0087	
AR0088	
AR0089	
AR0090	
AR0091	
AR0092	
AR0093	
AR0094	
AR0095	
AR0096	
AR0097	 excited version of AR0111
AR0098	
AR0099	
AR0100	

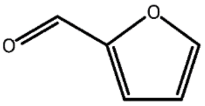
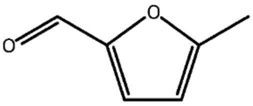
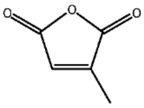
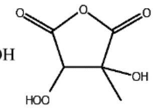
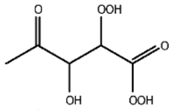
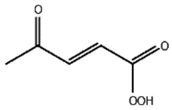
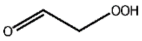
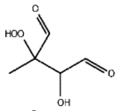
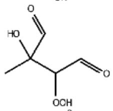
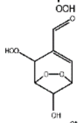
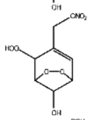
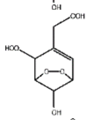
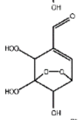
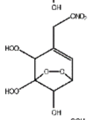
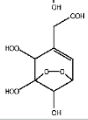
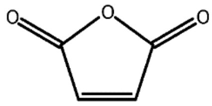
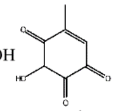
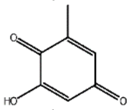
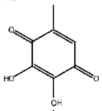
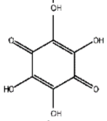
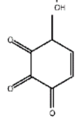
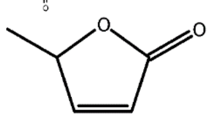
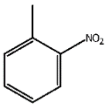
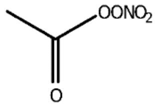
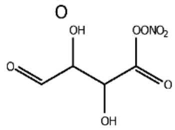
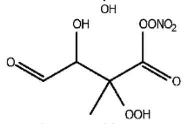
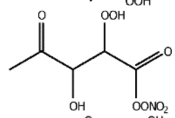
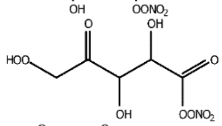
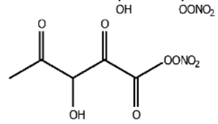
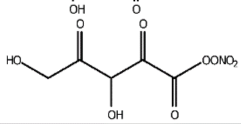
name	molecule (or position isomer)
AR0101	
AR0102	
AR0104	
AR0105	
AR0106	
AR0107	
AR0108	
AR0109	
AR0110	
AR0111	
AR0112	
AR0113	
AR0114	
AR0115	
AR0116	

name	molecule (or position isomer)
AR0117	
AR0118	
AR0119	
AR0120	
AR0121	
AR0124	
AR0125	
AR0126	
AR0127	
AR0128	
AR0129	
AR0130	
AR0131	
AR0132	
AR0133	

name	molecule (or position isomer)
AR0134	
AR0138	
AR0140	
AR01401O	
AR0140OOH	
AR0141	
AR0142	
AR0144	
AR0152	
AR0153	
AU4000	
AU5000	
AU5002	
AU50DN	
AU6000	

name	molecule (or position isomer)	
AU7000		
BTOL2OH1O		Same as AR0114 (intermediate model species use to simplify the mechanism)
BTOL3OH1O		
BTOL3OH2O		
BTOL3OHOOH		
BTOL4OH1O		
BTOL4OH2O		
BTOL4OHOOH		
BTOL5OH1O		
BTOL5OH2O		
BTOL5OHOOH		
BZALDOH		
C73K1OH2O		
C73K1OHOOH		
CH2O		

name	molecule (or position isomer)
D02000	
DD2000	
DD3000	
DD3001	
DD5002	
DK3000	
DK4000	
DK4001	
DK5000	
ED4001	
ED5000	
ED5000OOH	
ED5002OOH	
FUROH	
FURON	

name	molecule (or position isomer)
FURR3	
FURR5	
FURR6	
FURR6OHOOH	
GH5002	
GU5002	
HD2000	
HD5000	
HD5001	
HOM1O	
HOM1ONO2	
HOM1OOH	
HOM2O	
HOM2ONO2	
HOM2OOH	
MALAHY	
MBQN1K1OH	
MBQN1OH	
MBQN2OH	
MBQN3OH	
Me6Cy1U3K	
MFUR	
NTOL	
P02000	
PD5002	
PH5000	
PH5002	
PH5004	
PK5001	
PK5003	

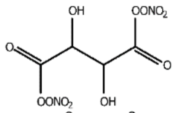
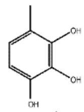
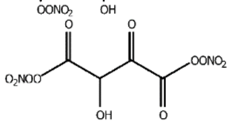
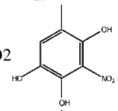
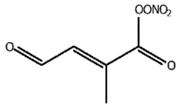
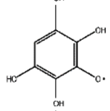
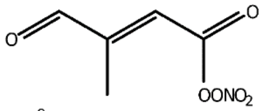
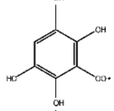
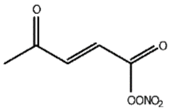
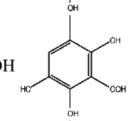
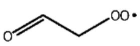
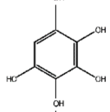
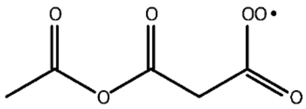
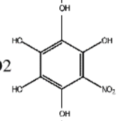
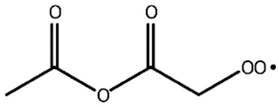
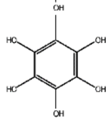
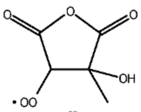
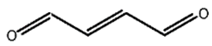
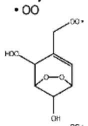
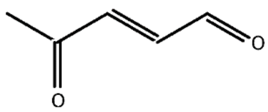
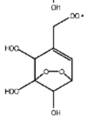
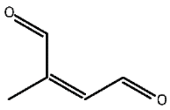
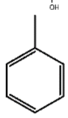
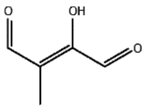
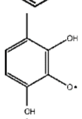
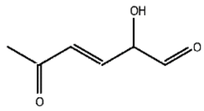
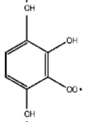
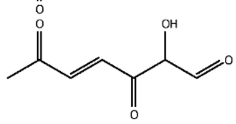
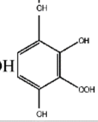
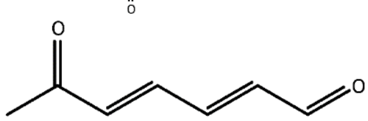
name	molecule (or position isomer)	name	molecule (or position isomer)
PP4000		TOL3OH	
PP4004		TOL3OH1NO2	
PU5000		TOL3OH1O	
PU5001		TOL3OH2O	
PU5002		TOL3OHOOH	
radED4001		TOL4OH	
radED5000		TOL4OH1NO2	
radED5002		TOL5OH	
radFURR6		UD4000	
radHOM7O		UD5000	
radHOM9O		UD5001	
TOL		UD5002	
TOL2OH1O		UD6000	
TOL2OH2O		UD7000	
TOL2OHOOH		UU7000	

Table S5: MG-Cr-Al chemical mechanism.

reaction ID	reaction			kinetic type	kinetic values
BLOC 0 : TOLUENE					
B0-001	TOL + HO	→	0.60 AR0086 + 0.07 AR0085 + .1674 AR0088 + 0.05 AR0087 + 0.10 UU7000 + .0126 NTOL	*ARR2*	1.814E-12 -338.
BLOC 1 : METHYL ATTACK PATHWAY					
B1-001	AR0085 + NO	→	0.89 AR0089 + 0.11 AR0090	*ARR2*	2.537E-12 -360.
B1-002	AR0085 + NO3	→	AR0089	*ARR1*	0.250E-11
B1-003	AR0085 + HO2	→	AR0091	*ARR2*	0.239E-12 -1300.
B1-004	AR0089	→	AR0102	*ARR2(O2)*	0.370E-13 460.
B1-005	AR0090	→	AR0089	*PHOTO*	2.2176E-06
B1-006	AR0090 + HO	→	AR0102	*ARR1*	0.603E-11
B1-007	AR0091	→	AR0089	*PHOTO*	6.3472E-06
B1-008	AR0091 + HO	→	AR0102	*ARR1*	0.205E-10
B1-009	AR0102 + HO	→	AR0120	*ARR1*	0.129E-10
B1-010	AR0102 + NO3	→	AR0120	*ARR1*	0.240E-14
B1-011	AR0102	→	AR0028	*PHOTO*	1.0557E-05
B1-012	AR0102	→	AR0120	*PHOTO*	1.0556E-05
B1-013	AR0120 + NO	→	AR0028	*ARR2*	0.810E-11 -270.
B1-014	AR0120 + NO3	→	AR0028	*ARR1*	0.400E-11
B1-015	AR0120 + NO2	→	AR0130	*TROE5*	0.270E-27 7.1 0.120E-10 0.9 0.3
B1-016	AR0120 + HO2	→	0.71 AR0131 + 0.29 AR0132	*ARR2*	0.430E-12 -1040.
B1-017	AR0130	→	AR0120	*TROE7*	0.328E-02 12100. 0.0 0.268E+17 13600. 0.0 0.3
B1-018	AR0130 + HO	→	AR0043	*ARR1*	0.106E-11
B1-019	AR0131	→	AR0028	*PHOTO*	6.3472E-06
B1-020	AR0131 + HO	→	AR0120	*ARR1*	0.466E-11
B1-021	AR0028 + NO	→	AR0013	*ARR2*	0.254E-11 -360.
B1-022	AR0028 + NO3	→	AR0013	*ARR1*	0.250E-11
B1-023	AR0028 + HO2	→	AR0043	*ARR1*	0.224E-12 -1300.
B1-024	AR0043	→	AR0013	*PHOTO*	6.3472E-06
B1-025	AR0043 + HO	→	AR0028	*ARR1*	0.360E-11
B1-026	AR0013 + NO2	→	AR0027	*ARR1*	0.208E-11
B1-027	AR0013 + O3	→	AR0028	*ARR1*	0.286E-12
B1-028	AR0027 + HO	→	AR0042	*ARR1*	0.900E-12
B1-029	AR0027 + NO3	→	AR0042	*ARR1*	0.900E-13
B1-030	AR0132 + HO	→	AR0028	*ARR1*	0.110E-11
BLOC 2 : CRESOL PATHWAY					
B2-001	AR0088 + HO	→	0.068 AR0098 + 0.186 AR0099 + 0.676 AR0100 + 0.07 BZALDOH	*ARR1*	4.649E-11
B2-002	AR0088 + NO3	→	0.39 AR0098 + 0.10 AR0099 + 0.51 AR0101	*ARR1*	1.250E-11
B2-003	AR0098 + O3	→	AR0112	*ARR1*	0.286E-12
B2-004	AR0098 + NO2	→	AR0113	*ARR1*	0.208E-11
B2-005	AR0099 + NO	→	AR0114	*ARR2*	0.254E-11 -360.
B2-006	AR0099 + NO3	→	AR0114	*ARR1*	0.250E-11
B2-007	AR0099 + HO2	→	0.35 AR0115 + 0.65 AR0114	*ARR2*	0.239E-12 -1300.
B2-008	AR0112 + NO	→	AR0098	*ARR2*	0.254E-11 -360.
B2-009	AR0112 + NO3	→	AR0098	*ARR1*	0.250E-11
B2-010	AR0112 + HO2	→	AR0125	*ARR2*	0.239E-12 -1300.
B2-011	AR0125 + HO	→	AR0112	*ARR1*	0.465E-10

B2-012	AR0125	→	AR0098	*PHOTO*	6.3472E-06	
B2-013	AR0113 + NO3	→	AR0126	*ARR1*	0.313E-12	
B2-014	AR0113 + HO	→	AR0126	*ARR1*	0.153E-11	
B2-015	AR0126 + NO2	→	AR0138	*ARR1*	0.208E-11	
B2-016	AR0114	→	0.32 AR0127 + 0.68 BTOL2OH1O	*ARR1*	1.0E+06	
B2-017	BTOL2OH1O	→	0.350 AU5002 + 0.350 DD2000 + 0.140 UD5002 + 0.140 DD2000 + 0.250 UD5000 + 0.250 AD2000 + 0.095 UD4000 + 0.095 AK3000 + 0.090 AU5000 + 0.090 DD2000 + 0.075 AU4000 + 0.075 DK3000	*ARR1*	1.0E+07	
B2-018	AR0115 + HO	→	AR0099	*ARR1*	0.115E-09	
B2-019	AR0115	→	AR0114	*PHOTO*	6.3472E-06	
B2-020	AR0101 + NO	→	AR0118	*ARR2*	0.254E-11	-360.
B2-021	AR0101 + NO3	→	AR0118	*ARR1*	0.250E-11	
B2-022	AR0101 + HO2	→	AR01192	*ARR2*	0.239E-12	-1300.
B2-023	AR0119	→	AR0118	*PHOTO*	6.3472E-06	
B2-024	AR0119 + HO	→	AR0101	*ARR1*	0.107E-09	
B2-025	AR0119	→	AR0114	*PHOTO*	1.0401E-06	
B2-026	AR0118	→	DD2000 + AU5002	*ARR1*	0.100E+07	
B2-027	AR0127 + HO	→	0.93 AR0140 + 0.07 Me6Cy1U3K	*ARR1*	0.235E-10	
B2-028	AR0140 + HO2	→	AR0140OOH	*ARR2*	0.239E-12	-1300.
B2-029	AR0140 + NO	→	AR01401O	*ARR2*	0.270E-11	-360.
B2-030	AR0140OOH + HO	→	MBQN1K1OH	*ARR1*	1.42E-10	
B2-031	AR01401O	→	C73K1OH2O	*ARR1*	1.00E+6	
B2-032	C73K1OH2O + HO2	→	0.44 DD5002 + 0.56 C73K1OHOOH	*ARR2*	5.20E-13	-980.
B2-033	C73K1OHOOH + HO	→	C73K1OH2O	*ARR1*	9.29E-11	
B2-034	C73K1OH2O + NO	→	DD5002	*ARR2*	7.50E-12	-290.
B2-035	AR0100 + HO	→	0.07 AR0116 + 0.065 MBQN1OH + 0.73 TOL3OH + 0.135 BTOL3OH2O	*ARR1*	0.205E-09	
B2-036	AR0100 + NO3	→	AR0116	*ARR1*	0.201E-09	
B2-037	AR0100 + O3	→	AR0117	*ARR1*	0.281E-16	
B2-038	AR0116 + NO2	→	AR0128	*ARR1*	0.208E-11	
B2-039	AR0116 + O3	→	AR0129	*ARR1*	0.286E-12	
B2-040	AR0128 + HO	→	AR0142	*ARR1*	0.683E-11	
B2-041	AR0128 + NO3	→	AR0142	*ARR1*	0.503E-11	
B2-042	AR0129 + HO2	→	AR01442	*ARR2*	0.239E-12	-1300.
B2-043	AR0129 + NO	→	AR0116	*ARR2*	0.254E-11	-360.
B2-044	AR0129 + NO3	→	AR0116	*ARR1*	0.250E-11	
B2-045	AR0144	→	AR0116	*PHOTO*	6.3472E-06	
B2-046	AR0144 + HO	→	AR0129	*ARR1*	0.205E-09	
B2-047	AR0142 + NO	→	AR0152	*ARR2*	0.254E-11	-360.
B2-048	AR0142 + NO3	→	AR0152	*ARR1*	0.250E-11	
B2-049	AR0142 + HO2	→	AR01532	*ARR2*	0.239E-12	-1300.
B2-050	AR0153	→	AR0152	*PHOTO*	6.3472E-06	
B2-051	AR0153 + HO	→	AR0142	*ARR2*	0.190E-11	-190.
B2-052	AR0152	→	AD2000 + AU50DN	*ARR1*	1.00E+6	
B2-053	AU50DN + HO	→	FURR6	*ARR2*	0.190E-11	-190.
B2-054	FURR6 + HO	→	radFURR6	*ARR1*	0.150E-11	
B2-055	radFURR6 + HO2	→	FURR6OHOOH	*ARR2*	0.204E-12	-1300.
B2-056	radFURR6 + NO	→	DK3000	*ARR2*	0.270E-11	-360.
B2-057	radFURR6 + NO3	→	DK3000	*ARR1*	0.230E-11	
B2-058	FURR6OHOOH + HO	→	radFURR6	*ARR1*	1.700E-11	

B2-059	TOL3OH + HO	→	0.07 TOL2OH1O + 0.07 MBQN2OH + 0.73 TOL4OH + 0.13 BTOL4OH2O	*ARR1*	2.5E-10
B2-060	TOL4OH + HO	→	0.07 TOL3OH1O + 0.07 MBQN3OH + 0.73 TOL5OH + 0.13 BTOL5OH2O	*ARR1*	2.5E-10
B2-061	TOL2OH1O + NO2	→	TOL3OH1NO2	*ARR1*	0.208E-11
B2-062	TOL2OH1O + O3	→	TOL2OH2O	*ARR1*	0.286E-12
B2-063	TOL2OH2O + HO2	→	TOL2OHOOH2	*ARR2*	0.239E-12 -1300.
B2-064	TOL2OH2O + NO	→	TOL2OH1O	*ARR2*	0.254E-11 -360.
B2-065	TOL2OH2O + NO3	→	TOL2OH1O	*ARR1*	0.250E-11
B2-066	TOL2OHOOH	→	TOL2OH1O	*PHOTO*	6.3472E-06
B2-067	TOL2OHOOH + HO	→	TOL2OH2O	*ARR1*	0.205E-09
B2-068	TOL3OH1O + NO2	→	TOL4OH1NO2	*ARR1*	0.208E-11
B2-069	TOL3OH1O + O3	→	TOL3OH2O	*ARR1*	0.286E-12
B2-070	TOL3OH2O + HO2	→	TOL3OHOOH2	*ARR2*	0.239E-12 -1300.
B2-071	TOL3OH2O + NO	→	TOL3OH1O	*ARR2*	0.254E-11 -360.
B2-072	TOL3OH2O + NO3	→	TOL3OH1O	*ARR1*	0.250E-11
B2-073	TOL3OHOOH	→	TOL3OH1O	*PHOTO*	6.3472E-06
B2-074	TOL3OHOOH + HO	→	TOL3OH2O	*ARR1*	0.205E-09
B2-075	BTOL3OH2O + HO2	→	0.65 BTOL3OH1O + 0.35 BTOL3OHOOH	*ARR2*	0.239E-12 -1300.
B2-076	BTOL3OH2O + NO3	→	BTOL3OH1O	*ARR1*	0.250E-11
B2-077	BTOL3OH2O + NO	→	BTOL3OH1O	*ARR2*	0.254E-11 -360.
B2-078	BTOL3OH1O	→	0.165 AD5000 + 0.165 DD2000 + 0.165 UD5000 + 0.165 AA2000 + 0.165 AU5000 + 0.165 AD2000 + 0.165 DK5000 + 0.165 DD2000 + 0.165 AD4000 + 0.165 DK3000 + 0.165 AU4000 + 0.165 AK3000	*ARR1*	1.0E+06
B2-079	BTOL3OHOOH	→	BTOL3OH1O	*PHOTO*	6.3472E-06
B2-080	BTOL3OHOOH + HO	→	BTOL3OH2O	*ARR1*	0.205E-09
B2-081	BTOL4OH2O + HO2	→	0.65 BTOL4OH1O + 0.35 BTOL4OHOOH	*ARR2*	0.239E-12 -1300.
B2-082	BTOL4OH2O + NO3	→	BTOL4OH1O	*ARR1*	0.250E-11
B2-083	BTOL4OH2O + NO	→	BTOL4OH1O	*ARR2*	0.254E-11 -360.
B2-084	BTOL4OH1O	→	0.250 AD4001 + 0.250 DK3000 + 0.250 AD5000 + 0.250 AD2000 + 0.250 AU5000 + 0.250 AA2000 + 0.250 AK5000 + 0.250 DD2000	*ARR1*	1.0E+06
B2-085	BTOL4OHOOH	→	BTOL4OH1O	*PHOTO*	6.3472E-06
B2-086	BTOL4OHOOH + HO	→	BTOL4OH2O	*ARR1*	0.205E-09
B2-087	BTOL5OH2O + HO2	→	0.65 BTOL5OH1O + 0.35 BTOL5OHOOH	*ARR2*	0.239E-12 -1300.
B2-088	BTOL5OH2O + NO3	→	BTOL5OH1O	*ARR1*	0.250E-11
B2-089	BTOL5OH2O + NO	→	BTOL5OH1O	*ARR2*	0.254E-11 -360.
B2-090	BTOL5OH1O	→	0.250 AD5000 + 0.250 AA2000 + 0.250 AA4000 + 0.250 DK3000 + 0.250 AD4001 + 0.250 AK3000 + 0.250 AK5000 + 0.250 AD2000	*ARR1*	1.0E+06
B2-091	BTOL5OHOOH	→	BTOL5OH1O	*PHOTO*	6.3472E-06
B2-092	BTOL5OHOOH + HO	→	BTOL5OH2O	*ARR1*	0.205E-09

BLOC 3 : BICYCLIC COMPOUND PATHWAY

B3-001	AR0086 + NO	→	0.89 AR0092 + 0.11 AR0093	*ARR2*	2.542E-12 -360.
B3-002	AR0086 + NO3	→	AR0092	*ARR1*	0.250E-11
B3-003	AR0086 + HO2	→	AR00942	*ARR2*	0.239E-12 -1300.
B3-004	AR0086	→	radHOM7O	*ARR2*	1.297E+03 3920.
B3-005	radHOM7O	→	radHOM9O	*ARR1*	0.5
B3-006	radHOM7O + NO	→	0.80 HOM1O + 0.20 HOM1ONO2	*ARR2*	2.7E-12 360.

B3-007	radHOM7O + HO2	→	HOM1OOH	*ARR2*	2.6E-13 1300.
B3-008	radHOM9O + NO	→	0.80 HOM2O + 0.20 HOM2ONO2	*ARR2*	2.7E-12 360.
B3-009	radHOM9O + HO2	→	HOM2OOH	*ARR2*	2.6E-13 1300.
B3-010	AR0092	→	0.15 UD5001 + 0.15 DD2000 + 0.15 UD5000 + 0.15 DD2000 + 0.05 MFUR + 0.05 DD2000 + 0.20 UD4000 + 0.20 DK3000 + 0.30 FURR5 + 0.30 CH2O + 0.15 FURR3 + 0.15 D02000	*ARR1*	1.00E+06
B3-011	FURR5 + HO	→	FUROH	*ARR1*	1.570E-10
B3-012	AR0094	→	AR0092	*PHOTO*	6.3472E-06
B3-013	AR0094 + HO	→	AR0104	*ARR1*	0.964E-10
B3-014	AR0093	→	AR0092	*PHOTO*	1.0401E-06
B3-015	AR0093 + HO	→	AR0104	*ARR1*	0.716E-10
B3-016	AR0104	→	DD2000 + 3U5002	*PHOTO*	1.0291E-06
B3-017	AR0104 + HO	→	DD2000 + 3U5002	*ARR1*	0.900E-10
B3-018	MFUR + HO	→	AR0121	*ARR1*	0.690E-10
B3-019	MFUR + NO3	→	AR0121	*ARR1*	0.100E-11
B3-020	MFUR + O3	→	AR0121	*ARR1*	0.800E-18
B3-021	FURON + HO	→	AR0035	*ARR1*	0.445E-10
B3-022	FURON + NO3	→	AR0035	*ARR1*	0.300E-12
B3-023	FURON + O3	→	AR0035	*ARR1*	0.220E-18
B3-024	AR0121 + NO	→	ED5000	*ARR2*	0.254E-11 -360.
B3-025	AR0121 + NO3	→	ED5000	*ARR1*	0.250E-11
B3-026	AR0121 + HO2	→	AR01342	*ARR2*	0.205E-12 -1300.
B3-027	AR0134	→	ED5000	*PHOTO*	6.3472E-06
B3-028	AR0134 + HO	→	AR0121	*ARR1*	0.253E-10
B3-029	ED5000 + HO	→	radED5000	*ARR1*	0.344E-10
B3-030	radED5000 + NO	→	radED5002	*ARR2*	0.750E-11 -290.
B3-031	radED5000 + HO2	→	0.56 ED5000OOH + 0.44 radED5002	*ARR2*	5.2E-13 -980.
B3-032	ED5000OOH + HO	→	radED5000	*ARR1*	3.59E-12
B3-033	radED5002 + NO	→	3K2000 + CH2O	*ARR2*	0.270E-11 -360.
B3-034	radED5002 + HO2	→	ED5002OOH2	*ARR2*	0.182E-12 -1300.
B3-035	ED5002OOH + HO	→	radED5002	*ARR1*	3.59E-12
B3-036	AR0035 + NO	→	ED4001	*ARR2*	0.254E-11 -360.
B3-037	AR0035 + NO3	→	ED4001	*ARR1*	0.250E-11
B3-038	AR0035 + HO2	→	AR0048	*ARR2*	0.205E-12 -1300.
B3-039	AR0048	→	ED4001	*PHOTO*	6.3472E-06
B3-040	AR0048 + HO	→	AR0035	*ARR1*	0.368E-10
B3-041	ED4001 + HO	→	radED4001	*ARR1*	0.344E-10
B3-042	radED4001 + NO	→	CH2O	*ARR2*	0.270E-11 -360.
B3-043	radED4001 + HO2	→	HD2000	*ARR2*	1.126E-13 -1300.
B3-044	HD2000 + HO	→	DD2000	*ARR1*	2.91E-11
BLOC 4 : RING OPENING PATHWAY (EPOX)					
B4-001	AR0087	→	AR0010 + 3K2000	*PHOTO*	7.565E-04
B4-002	AR0087	→	2U6000	*PHOTO*	7.565E-04
B4-003	AR0087 + NO3	→	AR0095	*ARR2*	0.396E-11 1862.
B4-004	AR0087 + HO	→	0.69 AR0096 + 0.31 AR0095	*ARR1*	0.800E-10
B4-005	AR0087 + O3	→	AR0010 + AR0097	*ARR1*	0.500E-17
B4-006	AR0095 + NO	→	2U6000	*ARR2*	0.810E-11 -270.
B4-007	AR0095 + NO2	→	AR0105	*TROE5*	0.270E-27 7.1 0.120E-10 0.9 0.3
B4-008	AR0095 + NO3	→	2U6000	*ARR1*	0.400E-11
B4-009	AR0095 + HO2	→	0.71 AR0106 + 0.29 AR01072	*ARR2*	0.430E-12 -1040.

B4-010	AR0105	→	AR0095	*TROE7*	0.490E-02 12100. 0.0 0.540E+17 13830. 0.0 0.3
B4-011	AR0105 + HO	→	UD5000	*ARR1*	0.596E-10
B4-012	AR0106	→	2U6000	*PHOTO*	6.3472E-06
B4-013	AR0106	→	2U6000	*PHOTO*	1.0557E-05
B4-014	AR0106	→	2U6000	*PHOTO*	1.0556E-05
B4-015	AR0106 + HO	→	AR0095	*ARR1*	0.629E-10
B4-016	AR0107	→	2U6000	*PHOTO*	1.0557E-05
B4-017	AR0107	→	2U6000	*PHOTO*	1.0556E-05
B4-018	AR0107 + HO	→	2U6000	*ARR1*	0.598E-10
B4-019	AR0096 + NO	→	0.89 AR0108 + 0.11 AR0109	*ARR2*	2.537E-12 -360.
B4-020	AR0096 + NO3	→	AR0108	*ARR1*	0.250E-11
B4-021	AR0096 + HO2	→	AR01102	*ARR2*	0.239E-12 -1300.
B4-022	AR0108	→	0.5 DK4000 + 0.5 DK3000 + 0.5 AR0010	*ARR1*	1.000E+06
B4-023	AR0109 + HO	→	AR0124	*ARR1*	0.306E-10
B4-024	AR0109	→	AR0010 + 3K2000	*PHOTO*	2.2690E-05
B4-025	AR0109	→	AR0010	*PHOTO*	1.0291E-06
B4-026	AR0110	→	AR0108	*PHOTO*	6.3472E-06
B4-027	AR0110	→	AR0108	*PHOTO*	2.2690E-05
B4-028	AR0110	→	AR0108	*PHOTO*	1.0291E-06
B4-029	AR0110 + HO	→	AR0124	*ARR1*	0.704E-10
B4-030	AR0010 + HO	→	AR0020	*ARR1*	0.432E-10
B4-031	AR0010 + NO3	→	AR0020	*ARR2*	0.115E-10 1862.
B4-032	AR0124	→	AR0010 + 3K2000	*PHOTO*	2.2690E-05
B4-033	AR0124	→	AR0010 + 3K2000	*PHOTO*	3.3377E-04
B4-034	AR0124 + HO	→	AR0010 + 3K2000	*ARR1*	0.406E-10
B4-035	AR0020 + NO2	→	AR0038	*TROE5*	0.270E-27 7.1 0.120E-10 0.9 0.3
B4-036	AR0020 + HO2	→	0.71 AR0039 + 0.29 AR00402	*ARR2*	0.430E-12 -1040.
B4-037	AR0038	→	AR0020	*TROE7*	0.490E-02 12100. 0.0 0.540E+17 13830. 0.0 0.3
B4-038	AR0038 + HO	→	DD3001	*ARR1*	0.229E-10
B4-039	AR0039 + HO	→	AR0020	*ARR1*	0.262E-10
B4-040	AR0097	→	0.18 AR0111 + .125 D02000 + 3K2000	*ARR1*	1.000E+06
B4-041	AR0111 + SO2	→	SULF + DK3000	*ARR1*	0.700E-13
B4-042	AR0111 + CO	→	DK3000	*ARR1*	0.120E-14
B4-043	AR0111 + NO	→	DK3000	*ARR1*	0.100E-13
B4-044	AR0111 + NO2	→	DK3000	*ARR1*	0.100E-14
B4-045	AR0111	→	.375 DK3000 + .625 AK3000	*ARR1*	1.600E-17
BLOC 5 : RING OPENING PATHWAY (ALCENE)					
B5-001	UU7000 + HO	→	0.32 3U7000 + 0.68 2U7000	*ARR1*	0.644E-10
B5-002	UU7000 + NO3	→	0.08 3U7000 + 0.92 2U7000	*ARR1*	2.0E-13
B5-003	UU7000	→	0.5 1U6000 + 0.5 3U7000	*PHOTO*	5.1086E-05
B5-004	2U7000 + NO	→	1U7000	*ARR2*	0.270E-11 -360.
B5-005	2U7000 + NO3	→	1U7000	*ARR1*	0.230E-11
B5-006	1U7000	→	0.125 UD7000 + 0.500 UD6000 + 0.125 UD4000 + 0.125 DK3000 + 0.125 UD5000 + 0.125 DD2000 + 0.125 UD5001 + 0.125 A02000	*ARR3*	0.112E+10 1.7 2851.
B5-007	3U7000 + NO	→	1U6000	*ARR2*	0.810E-11 -270.
B5-008	3U7000 + NO3	→	1U6000	*ARR1*	0.500E-11
B5-009	UD7000 + HO	→	2D7000	*ARR1*	0.426E-10
B5-010	AU7000 + HO	→	2D7000	*ARR1*	8.73E-11
B5-011	2D7000 + NO	→	1D7000	*ARR2*	0.270E-11 -360.
B5-012	2D7000 + HO2	→	AU70002	*ARR2*	0.281E-12 -1250.

B5-013	2D7000 + NO3	→	1D7000	*ARR1*	0.230E-11
B5-014	1D7000	→	0.05 AU5002 + 0.05 AD2000 + 0.35 AU4000 + 0.35 AK3000 + 0.35 DK4000 + 0.35 DK3000 + 0.25 DD3000 + 0.25 DK4001	*ARR3*	0.112E+10 1.7 2851.
B5-015	AU6000 + HO	→	2D6000	*ARR1*	2.89E-11
B5-016	UD6000 + HO	→	2D6001	*ARR1*	1.09E-10
B5-017	2D6000 + NO	→	1D6000	*ARR2*	2.703E-11 -360.
B5-018	2D6000 + HO2	→	DK4000 + AD20002	*ARR2*	0.264E-12 -1250.
B5-019	2D6000 + NO3	→	1D6000	*ARR1*	0.230E-11
B5-020	2D6001 + NO	→	1D6001	*ARR2*	2.703E-11 -360.
B5-021	2D6001 + HO2	→	AU60002	*ARR2*	0.264E-12 -1250.
B5-022	2D6001 + NO3	→	1D6001	*ARR1*	0.230E-11
B5-023	1D6000	→	AD2000 + DK4000	*ARR3*	0.112E+10 1.7 2451.
B5-024	1D6001	→	DK3000 + DD3000	*ARR3*	0.112E+10 1.7 2451.
BLOC 6 : OTHER MAJOR GAS COMPOUND FORMATION PATHWAY					
B6-001	UD4000 + HO	→	.144 2D4000	*ARR1*	5.207E-11
B6-002	UD4000 + O3	→	DD2000	*ARR1*	1.600E-18
B6-003	UD4000	→	FURON	*PHOTO*	8.7754E-04
B6-004	UD4000	→	MALAHY	*PHOTO*	8.7754E-04
B6-005	2U6000 + NO	→	0.90 1U6000	*ARR2*	2.703E-11 -360.
B6-006	2U6000 + NO3	→	1U6000	*ARR1*	0.230E-11
B6-007	2U6000 + MO2	→	0.34 1U6000 + 0.33 UD6000	*ARR2*	0.565E-13 -845.
B6-008	2U6000 + ACO3	→	0.65 1U6000	*ARR1*	0.100E-10
B6-009	1U6000	→	UD5000	*ARR3*	0.112E+10 1.7 2451.
B6-010	UD6000	→	UD5000	*PHOTO*	2.7986E-06
B6-011	UD5000 + HO	→	0.54 3U5002 + 0.23 FURR6 + 0.23 2D5003	*ARR1*	0.558E-10
B6-012	UD5000 + O3	→	0.50 DD2000 + 0.50 DK3000 + 3K2000	*ARR1*	0.480E-17
B6-013	UD5000 + NO3	→	3U5002	*ARR1*	0.107E-13
B6-014	UD5000	→	MFUR	*PHOTO*	1.1953E-03
B6-015	UD5000	→	MALAHY	*PHOTO*	1.1953E-03
B6-016	UD5001 + HO	→	0.40 3U5000 + 0.40 3U5001 + 0.10 2D5000 + 0.10 2D5001	*ARR1*	5.168E-11
B6-017	UD5001 + O3	→	0.30 DK3000 + 0.70 DD2000 + 3K2000	*ARR1*	1.600E-18
B6-018	UD5001 + NO3	→	0.50 3U5000 + 0.50 3U5001	*ARR1*	0.222E-13
B6-019	UD5001	→	FURON	*PHOTO*	8.7754E-04
B6-020	UD5001	→	MALAHY	*PHOTO*	8.7754E-04
B6-021	MALAHY + HO	→	AR0080	*ARR1*	0.150E-11
B6-022	3U5001 + NO	→	1D4001	*ARR2*	0.810E-11 -270.
B6-023	3U5001 + NO2	→	PU5001	*ARR3*	0.330E-08 -1.0 0.
B6-024	3U5001 + NO3	→	1D4001	*ARR1*	0.500E-11
B6-025	3U5001 + MO2	→	0.68 1D4001 + 0.31 AU5002	*ARR1*	0.100E-10
B6-026	3U5001 + ACO3	→	1D4001	*ARR2*	0.500E-11 -500.
B6-027	1D4001	→	DK3000	*ARR3*	0.224E+10 1.7 2567.
B6-028	2D5001 + NO	→	.967 1D5001	*ARR2*	0.270E-11 -360.
B6-029	2D5001 + HO2	→	HD50012	*ARR2*	0.242E-12 -1250.
B6-030	2D5001 + NO3	→	1D5001	*ARR1*	0.230E-11
B6-031	1D5001	→	DK3000 + DD2000	*ARR3*	0.112E+10 1.7 1890.
B6-032	2D5000 + NO	→	.967 1D5000	*ARR2*	0.270E-11 -360.
B6-033	2D5000 + HO2	→	HD5000	*ARR2*	0.242E-12 -1250.
B6-034	2D5000 + NO3	→	1D5000	*ARR1*	0.230E-11
B6-035	2D5000 + MO2	→	0.69 1D5000	*ARR2*	0.338E-12 415.

B6-036	2D5000 + ACO3	→	1D5000	*ARR1*	0.100E-10
B6-037	1D5000	→	DK3000 + DD2000	*ARR3*	0.112E+10 1.7 1734.
B6-038	DK3000	→	3K2000	*PHOTO*	9.5613E-05
B6-039	DK3000 + NO3	→	3K2000	*ARR2*	3.76E-12 1900.0
B6-040	DK3000 + HO	→	3K2000	*ARR2*	9.26E-13 -830.
B6-041	PU5001	→	3U5001	*ARR2*	0.200E+16 12800.
B6-042	PU5001 + O3	→	0.30 DK3000 + 3K2000	*ARR1*	0.480E-17
B6-043	PU5001	→	3U5001	*PHOTO*	5.9784E-07
B6-044	3K2000 + NO2	→	P02000	*TROE5*	0.850E-28 6.5 0.110E-10 1.0 0.6
B6-045	P02000	→	3K2000	*TROE7*	0.190E-02 12175. 0.0 0.280E+17 13580. 0.0 0.6
B6-046	P02000	→	3K2000	*PHOTO*	5.9784E-07
B6-047	1D4000	→	3K2000 + DD2000	*ARR3*	0.112E+10 1.7 2768.
B6-048	2D5003 + NO	→	1D5003	*ARR2*	0.261E-11 -360.
B6-049	2D5003 + NO3	→	1D5003	*ARR1*	0.230E-11
B6-050	1D5003	→	3K2000	*ARR3*	0.112E+10 1.7 2158.
B6-051	1D5003	→	DK3000 + DD2000	*ARR3*	0.112E+10 1.7 3197.
BLOC 7 : OTHER SOA MAJOR CONTRIBUTORS FORMATION PATHWAY					
B7-001	3U5002 + NO2	→	PU5002	*ARR3*	0.330E-08 -1.0 0.
B7-002	3U5002 + HO2	→	0.80 GU5002 + 0.20 AU50022	*ARR2*	0.640E-12 -925.
B7-003	3U5002 + NO	→	1D4000	*ARR2*	0.810E-11 -270.
B7-004	3U5002 + NO3	→	1D4000	*ARR1*	0.500E-11
B7-005	PU5002	→	3U5002	*ARR2*	0.200E+16 12800.
B7-006	PU5002 + HO	→	0.5 2P5006	*ARR1*	1.364E-11
B7-007	PU5002 + O3	→	0.50 DK3000 + 0.50 3K2000	*ARR1*	0.360E-17
B7-008	PU5002	→	3K2000	*PHOTO*	1.0009E-06
B7-009	PU5002	→	3U5002	*PHOTO*	5.9784E-07
B7-010	2P5006 + HO2	→	PH50022	*ARR2*	0.242E-12 -1250.
B7-011	2P5006 + NO	→	.967 1P5006	*ARR2*	0.270E-11 -360.
B7-012	2P5006 + NO3	→	1P5006	*ARR1*	0.230E-11
B7-013	PH5002	→	3H5004	*ARR2*	0.200E+16 12800.
B7-014	PH5002 + HO	→	.926 PK5001	*ARR1*	7.439E-11
B7-015	PH5002	→	3H5004	*PHOTO*	5.9784E-07
B7-016	PH5002	→	3K2000	*PHOTO*	2.0118E-06
B7-017	PH5002	→	1P5006	*PHOTO*	6.3472E-06
B7-018	1P5006	→	2P500A	*ARR2*	0.120E+12 3936.
B7-019	1P5006	→	PK5001	*ARR2(O2)*	0.250E-13 300.
B7-020	1P5006	→	DK3000	*ARR3*	0.112E+10 1.7 5234.
B7-021	PK5001	→	3K2000	*PHOTO*	2.0118E-06
B7-022	2P500A + HO2	→	PH50042	*ARR2*	0.242E-12 -1250.
B7-023	2P500A + NO	→	.967 1P500A	*ARR2*	0.270E-11 -360.
B7-024	2P500A + NO3	→	1P500A	*ARR1*	0.230E-11
B7-025	3H5004 + NO2	→	PH5002	*ARR3*	0.330E-08 -1.0 0.
B7-026	3H5004 + HO2	→	0.80 GH50022	*ARR2*	0.640E-12 -925.
B7-027	3H5004 + NO	→	DK4000	*ARR2*	0.810E-11 -270.
B7-028	3H5004 + NO3	→	DK4000	*ARR1*	0.500E-11
B7-029	3H5009 + NO2	→	PH5004	*ARR3*	0.330E-08 -1.0 0.
B7-030	PH5004	→	3H5009	*ARR2*	0.200E+16 12800.
B7-031	PH5004 + HO	→	.266 PD5002	*ARR1*	3.708E-11
B7-032	PH5004 + HO	→	2P500A	*ARR2*	0.191E-11 -190.
B7-033	PH5004	→	3H5009	*PHOTO*	5.9784E-07
B7-034	PH5004	→	1P500A	*PHOTO*	6.3472E-06

B7-035	3U5000 + NO2	→	PU5000	*ARR3*	0.330E-08 -1.0 0.
B7-036	3U5000 + NO	→	1D4000	*ARR2*	0.810E-11 -270.
B7-037	3U5000 + NO3	→	1D4000	*ARR1*	0.500E-11
B7-038	PU5000 + HO	→	0.13 2P5000	*ARR1*	0.283E-11
B7-039	PU5000	→	3U5000	*ARR2*	0.200E+16 12800.
B7-040	PU5000 + O3	→	0.70 DD2000	*ARR1*	0.480E-17
B7-041	PU5000	→	3U5000	*PHOTO*	5.9784E-07
B7-042	2P5000 + HO2	→	PH50002	*ARR2*	0.242E-12 -1250.
B7-043	3H5000 + NO2	→	PH5000	*ARR3*	0.330E-08 -1.0 0.
B7-044	3H5000 + NO	→	DK4000	*ARR2*	0.810E-11 -270.
B7-045	3H5000 + NO3	→	DK4000	*ARR1*	0.500E-11
B7-046	PH5000	→	3H5000	*ARR2*	0.200E+16 12800.
B7-047	PH5000 + HO	→	2P5000	*ARR2*	0.192E-11 -190.
B7-048	PH5000	→	3H5000	*PHOTO*	5.9784E-07
B7-049	GU5002 + HO	→	0.39 2G5006	*ARR1*	1.744E-11
B7-050	GU5002 + O3	→	0.5 DK3000 + 0.5 3K2000	*ARR1*	0.360E-17
B7-051	GU5002	→	3K2000	*PHOTO*	1.0009E-06
B7-052	GU5002	→	1D4000	*PHOTO*	6.3472E-06
B7-053	2G5006 + HO2	→	GH50022	*ARR2*	0.242E-12 -1250.
B7-054	GH5002	→	3K2000	*PHOTO*	2.0118E-06
B7-055	GH5002	→	DK4000	*PHOTO*	6.3472E-06
B7-056	AU5002 + O3	→	0.5 DK3000 + 0.5 3K2000	*ARR1*	0.360E-17
B7-057	1P500A	→	3P4000 +CH2O	*ARR3*	0.112E+10 1.7 3065.
B7-058	1P500A	→	PK5003	*ARR2*	0.400E+11 1661.
B7-059	PK5003	→	3K5003	*ARR2*	0.200E+16 12800.
B7-060	3K5003 + NO2	→	PK5003	*ARR3*	0.330E-08 -1.00.
B7-061	PD5002 + HO	→	0.43 3P4000	*ARR1*	0.481E-10
B7-062	PD5002 + NO3	→	0.64 3P4000	*ARR1*	1.005E-14
B7-063	PD5002	→	3P4000	*PHOTO*	8.1954E-05
B7-064	3P4000 + NO2	→	PP4000	*ARR3*	0.330E-08 -1.0 0.
B7-065	PP4000	→	3P4000	*ARR2*	0.400E+16 12800.
B7-066	PP4000 + HO	→	PP4004	*ARR1*	0.273E-10
B7-067	PP4000	→	3P4000	*PHOTO*	1.20E-06
B7-068	PP4004	→	3P400X	*ARR2*	0.400E+16 12800.
B7-069	3P400X + NO2	→	PP4004	*ARR3*	0.330E-08 -1.0 0.
B7-070	PP4004	→	3P400X	*PHOTO*	5.9784E-07
BLOC 8 : LOSS REACTIONS					
B8-001	NTOL + HO	→		*ARR1*	1.0E-12
B8-002	AR0027	→		*PHOTO*	1.23E-4
B8-003	BZALDOH + HO	→		*ARR1*	2.03E-11
B8-004	AR0113	→		*PHOTO*	5.0E-04
B8-005	AR0126 + O3	→		*ARR1*	0.286E-12
B8-006	AR0138 + HO	→		*ARR1*	5.10E-14
B8-007	AR0138 + NO3	→		*ARR1*	7.83E-15
B8-008	Me6Cy1U3K + HO	→		*ARR1*	4.78E-11
B8-009	AR0128	→		*PHOTO*	5.0E-04
B8-010	TOL3OH1NO2 + HO	→		*ARR1*	0.683E-11
B8-011	TOL3OH1NO2 + NO3	→		*ARR1*	0.503E-11
B8-012	TOL4OH1NO2 + HO	→		*ARR1*	0.683E-11
B8-013	TOL4OH1NO2 + NO3	→		*ARR1*	0.503E-11

B8-014	MBQN1OH + HO	→	*ARR1*	0.235E-10
B8-015	MBQN2OH + HO	→	*ARR1*	0.235E-10
B8-016	MBQN3OH + HO	→	*ARR1*	0.235E-10
B8-017	MBQN1OH + NO3	→	*ARR1*	0.100E-11
B8-018	MBQN2OH + NO3	→	*ARR1*	0.100E-11
B8-019	MBQN3OH + NO3	→	*ARR1*	0.100E-11
B8-020	TOL5OH + HO	→	*ARR1*	2.5E-10
B8-021	AU5000 + HO	→	*ARR1*	4.51E-11
B8-022	AU5000 + O3	→	*ARR1*	4.80E-18
B8-023	AU5000 + NO3	→	*ARR1*	1.91E-14
B8-024	UD5002 + HO	→	*ARR1*	4.51E-11
B8-025	UD5002 + O3	→	*ARR1*	4.80E-18
B8-026	UD5002 + NO3	→	*ARR1*	1.91E-14
B8-027	DD5002 + HO	→	*ARR1*	1.84E-11
B8-028	AD5000 + HO	→	*ARR1*	3.82E-11
B8-029	AD5000 + O3	→	*ARR1*	3.60E-18
B8-030	AD5000 + NO3	→	*ARR1*	8.35E-12
B8-031	DK5000 + HO	→	*ARR1*	3.82E-11
B8-032	DK5000 + O3	→	*ARR1*	3.60E-18
B8-033	DK5000 + NO3	→	*ARR1*	8.35E-12
B8-034	MBQN1K1OH + HO	→	*ARR1*	6.33E-11
B8-035	HOM1O + HO	→	*ARR1*	1.68E-10
B8-036	HOM2O + HO	→	*ARR1*	2.16E-10
B8-037	HOM1OOH + HO	→	*ARR1*	2.50E-10
B8-038	HOM2OOH + HO	→	*ARR1*	3.00E-10
B8-039	HOM1ONO2 + HO	→	*ARR1*	1.72E-10
B8-040	HOM2ONO2 + HO	→	*ARR1*	1.76E-10
B8-041	FURR5 + NO3	→	*ARR1*	4.500E-12
B8-042	FURR5 + O3	→	*ARR1*	7.000E-15
B8-043	FURR3 + HO	→	*ARR1*	1.330E-10
B8-044	FURR3 + NO3	→	*ARR1*	4.800E-12
B8-045	FURR3 + O3	→	*ARR1*	7.000E-15
B8-046	FUROH + HO	→	*ARR1*	1.570E-10
B8-047	FUROH + NO3	→	*ARR1*	4.500E-12
B8-048	FUROH + O3	→	*ARR1*	7.000E-15
B8-049	AR0104 + O3	→	*ARR1*	3.23E-17
B8-050	AR0104 + NO3	→	*ARR1*	4.27E-14
B8-051	AR0010	→	*PHOTO*	2.2690E-05
B8-052	AR0020 + NO	→	*ARR2*	0.810E-11 -270.
B8-053	AR0020 + NO3	→	*ARR1*	0.400E-11
B8-054	AR0039	→	*PHOTO*	6.3472E-06
B8-055	AR0039	→	*PHOTO*	2.2690E-05
B8-056	2U7000 + HO2	→	*ARR2*	0.281E-12 -1250.
B8-057	3U7000 + HO2	→	*ARR2*	0.640E-12 -925.
B8-058	AU5002 + HO	→	*ARR1*	2.19E-11
B8-059	AU4000 + HO	→	*ARR1*	3.28E-11
B8-060	A02000 + HO	→	*ARR2*	4.00E-14 -850.
B8-061	AK3000 + HO	→	*ARR2*	4.90E-14 -276.
B8-062	DK4000 + HO	→	*ARR1*	2.60E-11
B8-063	DD3000 + HO	→	*ARR1*	3.10E-11
B8-064	DK4001 + HO	→	*ARR1*	1.30E-11

B8-065	AD2000 + HO	→	*ARR1*	1.34E-11
B8-066	UD4000 + NO3	→	*ARR1*	0.149E-13
B8-067	2U6000 + HO2	→	*ARR2*	0.264E-12 -1250.
B8-068	HD5000 + HO	→	*ARR1*	0.510E-10
B8-069	HD5000 + NO3	→	*ARR1*	0.579E-12
B8-070	HD5001 + HO	→	*ARR1*	1.111E-10
B8-071	HD5001 + NO3	→	*ARR1*	0.683E-13
B8-072	CH2O	→	*PHOTO*	6.10E-05
B8-073	CH2O + HO	→	*ARR2*	0.860E-11 -20.
B8-074	CH2O + NO3	→	*ARR1*	0.580E-15
B8-075	PU5002 + NO3	→	*ARR1*	0.680E-14
B8-076	PU5002	→	*PHOTO*	1.0009E-05
B8-077	PK5001	→	*ARR2*	0.200E+16 12800.
B8-078	PK5001 + HO	→	*ARR1*	0.342E-11
B8-079	PK5001	→	*PHOTO*	8.1954E-05
B8-080	3H5009 + HO2	→	*ARR2*	0.640E-12 -925.
B8-081	3H5009 + NO	→	*ARR2*	0.810E-11 -270.
B8-082	3H5009 + NO3	→	*ARR1*	0.500E-11
B8-083	PH5004	→	*PHOTO*	2.0118E-06
B8-084	3U5000 + HO2	→	*ARR2*	0.640E-12 -925.
B8-085	PU5000 + NO3	→	*ARR1*	0.941E-13
B8-086	PU5000	→	*PHOTO*	1.9E-05
B8-087	2P5000 + NO	→	*ARR2*	0.270E-11 -360.
B8-088	2P5000 + NO3	→	*ARR1*	0.230E-11
B8-089	3H5000 + HO2	→	*ARR2*	0.640E-12 -925.
B8-090	PH5000 + HO	→	*ARR1*	2.626E-11
B8-091	PH5000 + NO3	→	*ARR1*	0.558E-12
B8-092	PH5000	→	*PHOTO*	9.14E-06
B8-093	GU5002 + NO3	→	*ARR1*	0.680E-14
B8-094	GU5002	→	*PHOTO*	1.0009E-05
B8-095	2G5006 + NO	→	*ARR2*	0.270E-11 -360.
B8-096	2G5006 + NO3	→	*ARR1*	0.230E-11
B8-097	GH5002 + HO	→	*ARR1*	7.795E-11
B8-098	GH5002	→	*PHOTO*	6.3472E-06
B8-099	AU5002 + NO3	→	*ARR1*	0.680E-14
B8-100	PK5003 + HO	→	*ARR1*	0.550E-11
B8-101	PK5003	→	*PHOTO*	8.40E-05
B8-102	3K5003 + HO2	→	*ARR2*	0.640E-12 -925.
B8-103	3K5003 + NO	→	*ARR2*	0.810E-11 -270.
B8-104	3K5003 + NO3	→	*ARR1*	0.500E-11
B8-105	PD5002	→	*ARR2*	0.200E+16 12800.
B8-106	PD5002	→	*PHOTO*	9.70E-06
B8-107	3P4000 + HO2	→	*ARR2*	0.640E-12 -925.
B8-108	3P4000 + NO	→	*ARR2*	0.810E-11 -270.
B8-109	3P4000 + NO3	→	*ARR1*	0.500E-11
B8-110	PP4004 + HO	→	*ARR1*	0.331E-11
B8-111	PP4004	→	*PHOTO*	8.1954E-05
B8-112	DD2000	→	*PHOTO*	8.0674E-05
B8-113	DD2000	→	*PHOTO*	4.1198E-06
B8-114	DD2000	→	*PHOTO*	7.6161E-06
B8-115	DD2000 + NO3	→	*ARR2*	2.90E-12 1900.0

B8-116	DD2000 + HO	→	*ARR1*	1.10E-11	
B8-117	PU5001 + HO	→	*ARR1*	0.283E-10	
B8-118	PU5001 + NO3	→	*ARR1*	0.941E-13	
B8-119	PU5001	→	*PHOTO*	6.4685E-06	
B8-120	PU5001	→	*PHOTO*	6.2783E-06	
B8-121	PU5001	→	*PHOTO*	6.2783E-06	
B8-122	3K2000 + HO2	→	*ARR2*	0.640E-12	-925.
B8-123	3K2000 + NO	→	*ARR2*	0.810E-11	-270.
B8-124	3K2000 + NO3	→	*ARR1*	0.500E-11	
B8-125	P02000 + HO	→	*ARR1*	0.102E-12	
B8-126	2D5003 + HO2	→	*ARR2*	0.242E-12	-1250.
B8-127	AA2000 + HO	→	*ARR2*	5.740E-14	-880.
B8-128	AD4000 + HO	→	*ARR1*	2.58E-11	
B8-129	AD4000 + NO3	→	*ARR1*	3.40E-13	
B8-130	AD4001 + HO	→	*ARR1*	2.58E-11	
B8-131	AD4001 + NO3	→	*ARR1*	3.40E-13	
B8-132	AK5000 + HO	→	*ARR1*	4.69E-11	
B8-133	AK5000 + NO3	→	*ARR1*	8.03E-15	
B8-134	AA4000 + HO	→	*ARR1*	2.58E-11	
B8-135	AA4000 + NO3	→	*ARR1*	3.40E-13	

Table S6 : kinetics.

kinetic type	formula
ARR1	$k = x_1$
ARR2	$k = x_1 \ e^{\frac{-x_2}{T}}$
ARR2(O2)	$k = x_1 \ e^{\frac{-x_2}{T}} \ [O_2]$
ARR3	$k = x_1 \ T^{x_2} \ e^{\frac{-x_3}{T}}$
TROE5	$k = \frac{k_0 \ [M]}{1+r} \times x_5^{\left(\frac{1}{1+(\log(r))^2}\right)}$ $r = \frac{k_0 \ [M]}{k_{inf}}$ $k_0 = x_1 \ e^{\frac{-x_2}{T}}$ $k_{inf} = x_3 \ e^{\frac{-x_4}{T}}$
TROE7	$k = \frac{k_0 \ [M]}{1+r} \times x_7^{\left(\frac{1}{1+(\log(r))^2}\right)}$ $r = \frac{k_0 \ [M]}{k_{inf}}$ $k_0 = x_1 \ T^{x_2} \ e^{\frac{-x_3}{T}}$ $k_{inf} = x_4 \ T^{x_5} \ e^{\frac{-x_6}{T}}$
PHOTO	$k = x_1$ (value associated to experimental UV lamps see table S7 for atmospheric values depending on zenithal angles)

Table S7: atmospheric photolysis rates of MG-Cr-Al mechanism.

reaction ID	reaction			atmospheric photolysis rates at sea level for the following zenithal angles: 0, 10, 20, 30, 40, 50, 60, 70, 78, 86, 90.										
B1-005	AR0090	→	AR0089	2.3428E-06	2.2921E-06	2.1428E-06	1.9015E-06	1.5810E-06	1.2023E-06	7.9880E-07	4.2341E-07	1.9324E-07	5.2977E-08	0.0000E+00
B1-007	AR0091	→	AR0089	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B1-011	AR0102	→	AR0028	4.9477E-06	4.8766E-06	4.6626E-06	4.2997E-06	3.7803E-06	3.0985E-06	2.2631E-06	1.3382E-06	6.6756E-07	2.0257E-07	0.0000E+00
B1-012	AR0102	→	AR0120	4.9470E-06	4.8759E-06	4.6620E-06	4.2992E-06	3.7800E-06	3.0984E-06	2.2630E-06	1.3382E-06	6.6755E-07	2.0257E-07	0.0000E+00
B1-019	AR0131	→	AR0028	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B1-024	AR0043	→	AR0013	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-012	AR0125	→	AR0098	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-019	AR0115	→	AR0114	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-023	AR0119	→	AR0118	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-025	AR0119	→	AR0114	2.6247E-06	2.5603E-06	2.3712E-06	2.0683E-06	1.6725E-06	1.2176E-06	7.5613E-07	3.6238E-07	1.4906E-07	3.4614E-08	0.0000E+00
B2-045	AR0144	→	AR0116	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-050	AR0153	→	AR0152	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-066	TOL2OHOOH	→	TOL2OH1O	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-073	TOL3OHOOH	→	TOL3OH1O	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-079	BTOL3OHOOH	→	BTOL3OH1O	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-085	BTOL4OHOOH	→	BTOL4OH1O	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B2-091	BTOL5OHOOH	→	BTOL5OH1O	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B3-012	AR0094	→	AR0092	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B3-014	AR0093	→	AR0092	2.6247E-06	2.5603E-06	2.3712E-06	2.0683E-06	1.6725E-06	1.2176E-06	7.5613E-07	3.6238E-07	1.4906E-07	3.4614E-08	0.0000E+00
B3-016	AR0104	→	DD2000 + 3U5002	3.5040E-06	3.4163E-06	3.1587E-06	2.7458E-06	2.2064E-06	1.5881E-06	9.6628E-07	4.4655E-07	1.7521E-07	3.7601E-08	0.0000E+00
B3-027	AR0134	→	ED5000	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B3-039	AR0048	→	ED4001	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B4-001	AR0087	→	AR0010 + 3K2000	4.2133E-03	4.1616E-03	4.0054E-03	3.7377E-03	3.3478E-03	2.8206E-03	2.1419E-03	1.3273E-03	6.7405E-04	2.0948E-04	0.0000E+00
B4-002	AR0087	→	2U6000	4.2133E-03	4.1616E-03	4.0054E-03	3.7377E-03	3.3478E-03	2.8206E-03	2.1419E-03	1.3273E-03	6.7405E-04	2.0948E-04	0.0000E+00
B4-012	AR0106	→	2U6000	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B4-013	AR0106	→	2U6000	4.9477E-06	4.8766E-06	4.6626E-06	4.2997E-06	3.7803E-06	3.0985E-06	2.2631E-06	1.3382E-06	6.6756E-07	2.0257E-07	0.0000E+00

B4-014	AR0106	→	2U6000	4.9470E-06	4.8759E-06	4.6620E-06	4.2992E-06	3.7800E-06	3.0984E-06	2.2630E-06	1.3382E-06	6.6755E-07	2.0257E-07	0.0000E+00
B4-016	AR0107	→	2U6000	4.9477E-06	4.8766E-06	4.6626E-06	4.2997E-06	3.7803E-06	3.0985E-06	2.2631E-06	1.3382E-06	6.6756E-07	2.0257E-07	0.0000E+00
B4-017	AR0107	→	2U6000	4.9470E-06	4.8759E-06	4.6620E-06	4.2992E-06	3.7800E-06	3.0984E-06	2.2630E-06	1.3382E-06	6.6755E-07	2.0257E-07	0.0000E+00
B4-024	AR0109	→	AR0010 + 3K2000	4.7518E-05	4.6558E-05	4.3706E-05	3.9012E-05	3.2618E-05	2.4837E-05	1.6330E-05	8.3723E-06	3.6409E-06	8.8371E-07	0.0000E+00
B4-025	AR0109	→	AR0010	3.5040E-06	3.4163E-06	3.1587E-06	2.7458E-06	2.2064E-06	1.5881E-06	9.6628E-07	4.4655E-07	1.7521E-07	3.7601E-08	0.0000E+00
B4-026	AR0110	→	AR0108	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B4-027	AR0110	→	AR0108	4.7518E-05	4.6558E-05	4.3706E-05	3.9012E-05	3.2618E-05	2.4837E-05	1.6330E-05	8.3723E-06	3.6409E-06	8.8371E-07	0.0000E+00
B4-028	AR0110	→	AR0108	3.5040E-06	3.4163E-06	3.1587E-06	2.7458E-06	2.2064E-06	1.5881E-06	9.6628E-07	4.4655E-07	1.7521E-07	3.7601E-08	0.0000E+00
B4-032	AR0124	→	AR0010 + 3K2000	4.7518E-05	4.6558E-05	4.3706E-05	3.9012E-05	3.2618E-05	2.4837E-05	1.6330E-05	8.3723E-06	3.6409E-06	8.8371E-07	0.0000E+00
B4-033	AR0124	→	AR0010 + 3K2000	2.3733E-04	2.3449E-04	2.2592E-04	2.1124E-04	1.8985E-04	1.6085E-04	1.2324E-04	7.7278E-05	3.9313E-05	1.2097E-05	0.0000E+00
B5-003	UU7000	→	0.5 1U6000 + 0.5 3U7000	6.1120E-05	5.9787E-05	5.5856E-05	4.9496E-05	4.1040E-05	3.1045E-05	2.0431E-05	1.0667E-05	4.8105E-06	1.2849E-06	0.0000E+00
B6-003	UD4000	→	FURON	4.8875E-04	4.8275E-04	4.6463E-04	4.3358E-04	3.8835E-04	3.2719E-04	2.4847E-04	1.5397E-04	7.8188E-05	2.4300E-05	0.0000E+00
B6-004	UD4000	→	MALAHY	4.8875E-04	4.8275E-04	4.6463E-04	4.3358E-04	3.8835E-04	3.2719E-04	2.4847E-04	1.5397E-04	7.8188E-05	2.4300E-05	0.0000E+00
B6-010	UD6000	→	UD5000	9.4770E-06	9.2366E-06	8.5314E-06	7.4036E-06	5.9347E-06	4.2580E-06	2.5810E-06	1.1880E-06	4.6507E-07	9.9632E-08	0.0000E+00
B6-014	UD5000	→	MFUR	6.6571E-04	6.5754E-04	6.3285E-04	5.9056E-04	5.2896E-04	4.4566E-04	3.3843E-04	2.0971E-04	1.0650E-04	3.3098E-05	0.0000E+00
B6-015	UD5000	→	MALAHY	6.6571E-04	6.5754E-04	6.3285E-04	5.9056E-04	5.2896E-04	4.4566E-04	3.3843E-04	2.0971E-04	1.0650E-04	3.3098E-05	0.0000E+00
B6-019	UD5001	→	FURON	4.8875E-04	4.8275E-04	4.6463E-04	4.3358E-04	3.8835E-04	3.2719E-04	2.4847E-04	1.5397E-04	7.8188E-05	2.4300E-05	0.0000E+00
B6-020	UD5001	→	MALAHY	4.8875E-04	4.8275E-04	4.6463E-04	4.3358E-04	3.8835E-04	3.2719E-04	2.4847E-04	1.5397E-04	7.8188E-05	2.4300E-05	0.0000E+00
B6-038	DK3000	→	3K2000	7.6968E-05	7.5838E-05	7.2455E-05	6.6780E-05	5.8776E-05	4.8426E-05	3.5847E-05	2.1662E-05	1.0736E-05	3.1607E-06	0.0000E+00
B6-043	PU5001	→	3U5001	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B6-046	P02000	→	3K2000	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B7-008	PU5002	→	3K2000	4.7467E-07	4.6782E-07	4.4722E-07	4.1230E-07	3.6239E-07	2.9696E-07	2.1687E-07	1.2826E-07	6.3971E-08	1.9414E-08	0.0000E+00
B7-009	PU5002	→	3U5002	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B7-015	PH5002	→	3H5004	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B7-016	PH5002	→	3K2000	3.2931E-06	3.2172E-06	2.9944E-06	2.6364E-06	2.1655E-06	1.6171E-06	1.0461E-06	5.3456E-07	2.3663E-07	6.1208E-08	0.0000E+00
B7-017	PH5002	→	1P5006	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B7-021	PK5001	→	3K2000	3.2931E-06	3.2172E-06	2.9944E-06	2.6364E-06	2.1655E-06	1.6171E-06	1.0461E-06	5.3456E-07	2.3663E-07	6.1208E-08	0.0000E+00
B7-033	PH5004	→	3H5009	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B7-034	PH5004	→	1P500A	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B7-041	PU5000	→	3U5000	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B7-048	PH5000	→	3H5000	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00

B7-051	GU5002	→	3K2000	4.7467E-07	4.6782E-07	4.4722E-07	4.1230E-07	3.6239E-07	2.9696E-07	2.1687E-07	1.2826E-07	6.3971E-08	1.9414E-08	0.0000E+00
B7-052	GU5002	→	1D4000	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B7-054	GH5002	→	3K2000	3.2931E-06	3.2172E-06	2.9944E-06	2.6364E-06	2.1655E-06	1.6171E-06	1.0461E-06	5.3456E-07	2.3663E-07	6.1208E-08	0.0000E+00
B7-055	GH5002	→	DK4000	5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B7-063	PD5002	→	3P4000	7.6968E-05	7.5838E-05	7.2455E-05	6.6780E-05	5.8776E-05	4.8426E-05	3.5847E-05	2.1662E-05	1.0736E-05	3.1607E-06	0.0000E+00
B7-067	PP4000	→	3P4000	1.6060E-06	1.5710E-06	1.4670E-06	1.3000E-06	1.0740E-06	8.1000E-07	5.3030E-07	2.7400E-07	1.2200E-07	3.1750E-08	0.0000E+00
B7-070	PP4004	→	3P400X	8.0298E-07	7.8532E-07	7.3328E-07	6.4911E-07	5.3727E-07	4.0517E-07	2.6517E-07	1.3707E-07	6.0989E-08	1.5874E-08	0.0000E+00
B8-002	AR0027	→		7.6968E-05	7.5838E-05	7.2455E-05	6.6780E-05	5.8776E-05	4.8426E-05	3.5847E-05	2.1662E-05	1.0736E-05	3.1607E-06	0.0000E+00
B8-004	AR0113	→		2.3733E-04	2.3449E-04	2.2592E-04	2.1124E-04	1.8985E-04	1.6085E-04	1.2324E-04	7.7278E-05	3.9313E-05	1.2097E-05	0.0000E+00
B8-009	AR0128	→		2.3733E-04	2.3449E-04	2.2592E-04	2.1124E-04	1.8985E-04	1.6085E-04	1.2324E-04	7.7278E-05	3.9313E-05	1.2097E-05	0.0000E+00
B8-051	AR0010	→		4.7518E-05	4.6558E-05	4.3706E-05	3.9012E-05	3.2618E-05	2.4837E-05	1.6330E-05	8.3723E-06	3.6409E-06	8.8371E-07	0.0000E+00
B8-054	AR0039	→		5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B8-055	AR0039	→		4.7518E-05	4.6558E-05	4.3706E-05	3.9012E-05	3.2618E-05	2.4837E-05	1.6330E-05	8.3723E-06	3.6409E-06	8.8371E-07	0.0000E+00
B8-072	CH2O	→		6.8710E-05	6.7475E-05	6.3788E-05	5.766Ee-05	4.9187E-05	3.8601E-05	2.6545E-05	1.4525E-05	6.7686E-06	1.8278E-06	0.0000E+00
B8-076	PU5002	→		4.7467E-06	4.6782E-06	4.4722E-06	4.1230E-06	3.6239E-06	2.9696E-06	2.1687E-06	1.2826E-06	6.3971E-07	1.9414E-07	0.0000E+00
B8-079	PK5001	→		7.6968E-05	7.5838E-05	7.2455E-05	6.6780E-05	5.8776E-05	4.8426E-05	3.5847E-05	2.1662E-05	1.0736E-05	3.1607E-06	0.0000E+00
B8-083	PH5004	→		3.2931E-06	3.2172E-06	2.9944E-06	2.6364E-06	2.1655E-06	1.6171E-06	1.0461E-06	5.3456E-07	2.3663E-07	6.1208E-08	0.0000E+00
B8-086	PU5000	→		8.6282E-06	8.5040E-06	8.1303E-06	7.4964E-06	6.5900E-06	5.4009E-06	3.9442E-06	2.3329E-06	1.1651E-06	3.5431E-07	0.0000E+00
B8-092	PH5000	→		2.3927E-05	1.4130E-05	1.3153E-05	1.1576E-05	9.4902E-06	7.0482E-06	4.5048E-06	2.2484E-06	9.6452E-07	2.3922E-07	0.0000E+00
B8-094	GU5002	→		4.7467E-06	4.6782E-06	4.4722E-06	4.1230E-06	3.6239E-06	2.9696E-06	2.1687E-06	1.2826E-06	6.3971E-07	1.9414E-07	0.0000E+00
B8-098	GH5002	→		5.0785E-06	4.9861E-06	4.7112E-06	4.2564E-06	3.6304E-06	2.8533E-06	1.9717E-06	1.0900E-06	5.1457E-07	1.4442E-07	0.0000E+00
B8-101	PK5003	→		8.0261E-05	7.9055E-05	7.5449E-05	6.9416E-05	6.0941E-05	5.0043E-05	3.6893E-05	2.2197E-05	1.0973E-05	3.2219E-06	0.0000E+00
B8-106	PD5002	→		8.5400E-06	8.4200E-06	8.0500E-06	7.4200E-06	6.5300E-06	5.4000E-06	4.0000E-06	2.4000E-06	1.1900E-06	3.5000E-07	0.0000E+00
B8-111	PP4004	→		7.6968E-05	7.5838E-05	7.2455E-05	6.6780E-05	5.8776E-05	4.8426E-05	3.5847E-05	2.1662E-05	1.0736E-05	3.1607E-06	0.0000E+00
B8-112	DD2000	→		4.4037E-06	4.3088E-06	4.0280E-06	3.5702E-06	2.9552E-06	2.2207E-06	1.4365E-06	7.2308E-07	3.1019E-07	7.4586E-08	0.0000E+00
B8-113	DD2000	→		3.2716E-05	3.2197E-05	3.0644E-05	2.8043E-05	2.4392E-05	1.9722E-05	1.4180E-05	8.2364E-06	3.9854E-06	1.1449E-06	0.0000E+00
B8-114	DD2000	→		1.8343E-05	1.7972E-05	1.6870E-05	1.5061E-05	1.2604E-05	9.6214E-06	6.3626E-06	3.2994E-06	1.4538E-06	3.6451E-07	0.0000E+00
B8-119	PU5001	→		2.9336E-06	2.8914E-06	2.7643E-06	2.5488E-06	2.2406E-06	1.8363E-06	1.3410E-06	7.9317E-07	3.9615E-07	1.2047E-07	0.0000E+00
B8-120	PU5001	→		2.8473E-06	2.8063E-06	2.6830E-06	2.4738E-06	2.1747E-06	1.7823E-06	1.3016E-06	7.6984E-07	3.8450E-07	1.1692E-07	0.0000E+00
B8-121	PU5001	→		2.8473E-06	2.8063E-06	2.6830E-06	2.4738E-06	2.1747E-06	1.7823E-06	1.3016E-06	7.6984E-07	3.8450E-07	1.1692E-07	0.0000E+00

Table S8: list of changes between MG, MG-Cr and MG-Cr-Al mechanism (not including losses reactions).

reaction ID	MG			MG-Cr			MG-Cr-Al		
B0-001	TOL + HO	→	0.65 AR0086 + 0.07 AR0085 + 0.18 AR0088 + 0.10 AR0087	TOL + HO	→	0.65 AR0086 + 0.07 AR0085 + 0.18 AR0088 + 0.10 AR0087	TOL + HO	→	0.60 AR0086 + 0.07 AR0085 + .1674 AR0088 + 0.05 AR0087 + 0.10 UU7000 + .0126 NTOL
B2-001	AR0088 + HO	→	0.073 AR0098 + 0.20 AR0099 + 0.727 AR0100	AR0088 + HO	→	0.073 AR0098 + 0.20 AR0099 + 0.727 AR0100	AR0088 + HO	→	0.068 AR0098 + 0.186 AR0099 + 0.676 AR0100 + 0.07 BZALDOH
B2-007	AR0099 + HO2	→	AR0115	AR0099 + HO2	→	0.35 AR0115 + 0.65 AR0114	AR0099 + HO2	→	0.35 AR0115 + 0.65 AR0114
B2-016	AR0114	→	0.32 AR0127 + 0.68 AU5002 + 0.68 DD2000	AR0114	→	0.32 AR0127 + 0.68 BTOL2OH1O	AR0114	→	0.32 AR0127 + 0.68 BTOL2OH1O
B2-017				BTOL2OH1O	→	0.350 AU5002 + 0.350 DD2000 + 0.140 UD5002 + 0.140 DD2000 + 0.250 UD5000 + 0.250 AD2000 + 0.095 UD4000 + 0.095 AK3000 + 0.090 AU5000 + 0.090 DD2000 + 0.075 AU4000 + 0.075 DK3000	BTOL2OH1O	→	0.350 AU5002 + 0.350 DD2000 + 0.140 UD5002 + 0.140 DD2000 + 0.250 UD5000 + 0.250 AD2000 + 0.095 UD4000 + 0.095 AK3000 + 0.090 AU5000 + 0.090 DD2000 + 0.075 AU4000 + 0.075 DK3000
B2-027	AR0127 + HO	→	AR0140	AR0127 + HO	→	AR0140	AR0127 + HO	→	0.93 AR0140 + 0.07 Me6Cy1U3K
B2-035	AR0100 + HO	→	AR0116	AR0100 + HO	→	0.07 AR0116 + 0.065 MBQN1OH + 0.73 TOL3OH + 0.135 BTOL3OH2O	AR0100 + HO	→	0.07 AR0116 + 0.065 MBQN1OH + 0.73 TOL3OH + 0.135 BTOL3OH2O
B2-052	AR0152	→	AD2000	AR0152	→	AD2000	AR0152	→	AD2000 + AU50DN
B2-053							AU50DN + HO	→	FURR6
B2-054							FURR6 + HO	→	radFURR6
B2-055							radFURR6 + HO2	→	FURR6OHOOH
B2-056							radFURR6 + NO	→	DK3000
B2-057							radFURR6 + NO3	→	DK3000
B2-058							FURR6OHOOH + HO	→	radFURR6
B2-059				TOL3OH + HO	→	0.07 TOL2OH1O + 0.07 MBQN2OH + 0.73 TOL4OH + 0.13 BTOL4OH2O	TOL3OH + HO	→	0.07 TOL2OH1O + 0.07 MBQN2OH + 0.73 TOL4OH + 0.13 BTOL4OH2O
B2-060				TOL4OH + HO	→	0.07 TOL3OH1O + 0.07 MBQN3OH + 0.73 TOL5OH + 0.13 BTOL5OH2O	TOL4OH + HO	→	0.07 TOL3OH1O + 0.07 MBQN3OH + 0.73 TOL5OH + 0.13 BTOL5OH2O
B2-061				TOL2OH1O + NO2	→	TOL3OH1NO2	TOL2OH1O + NO2	→	TOL3OH1NO2
B2-062				TOL2OH1O + O3	→	TOL2OH2O	TOL2OH1O + O3	→	TOL2OH2O
B2-063				TOL2OH2O + HO2	→	TOL2OHOOH	TOL2OH2O + HO2	→	TOL2OHOOH2
B2-064				TOL2OH2O + NO	→	TOL2OH1O	TOL2OH2O + NO	→	TOL2OH1O
B2-065				TOL2OH2O + NO3	→	TOL2OH1O	TOL2OH2O + NO3	→	TOL2OH1O

reaction ID	MG	MG-Cr			MG-Cr-Al		
B2-066		TOL2OHOOH	→	TOL2OH1O	TOL2OHOOH	→	TOL2OH1O
B2-067		TOL2OHOOH + HO	→	TOL2OH2O	TOL2OHOOH + HO	→	TOL2OH2O
B2-068		TOL3OH1O + NO2	→	TOL4OH1NO2	TOL3OH1O + NO2	→	TOL4OH1NO2
B2-069		TOL3OH1O + O3	→	TOL3OH2O	TOL3OH1O + O3	→	TOL3OH2O
B2-070		TOL3OH2O + HO2	→	TOL3OHOOH	TOL3OH2O + HO2	→	TOL3OHOOH2
B2-071		TOL3OH2O + NO	→	TOL3OH1O	TOL3OH2O + NO	→	TOL3OH1O
B2-072		TOL3OH2O + NO3	→	TOL3OH1O	TOL3OH2O + NO3	→	TOL3OH1O
B2-073		TOL3OHOOH	→	TOL3OH1O	TOL3OHOOH	→	TOL3OH1O
B2-074		TOL3OHOOH + HO	→	TOL3OH2O	TOL3OHOOH + HO	→	TOL3OH2O
B2-075		BTOL3OH2O + HO2	→	0.65 BTOL3OH1O + 0.35 BTOL3OHOOH	BTOL3OH2O + HO2	→	0.65 BTOL3OH1O + 0.35 BTOL3OHOOH
B2-076		BTOL3OH2O + NO3	→	BTOL3OH1O	BTOL3OH2O + NO3	→	BTOL3OH1O
B2-077		BTOL3OH2O + NO	→	BTOL3OH1O	BTOL3OH2O + NO	→	BTOL3OH1O
B2-078		BTOL3OH1O	→	0.165 AD5000 + 0.165 DD2000 + 0.165 UD5000 + 0.165 AA2000 + 0.165 AU5000 + 0.165 AD2000 + 0.165 DK5000 + 0.165 DD2000 + 0.165 AD4000 + 0.165 DK3000 + 0.165 AU4000 + 0.165 AK3000	BTOL3OH1O	→	0.165 AD5000 + 0.165 DD2000 + 0.165 UD5000 + 0.165 AA2000 + 0.165 AU5000 + 0.165 AD2000 + 0.165 DK5000 + 0.165 DD2000 + 0.165 AD4000 + 0.165 DK3000 + 0.165 AU4000 + 0.165 AK3000
B2-079		BTOL3OHOOH	→	BTOL3OH1O	BTOL3OHOOH	→	BTOL3OH1O
B2-080		BTOL3OHOOH + HO	→	BTOL3OH2O	BTOL3OHOOH + HO	→	BTOL3OH2O
B2-081		BTOL4OH2O + HO2	→	0.65 BTOL4OH1O + 0.35 BTOL4OHOOH	BTOL4OH2O + HO2	→	0.65 BTOL4OH1O + 0.35 BTOL4OHOOH
B2-082		BTOL4OH2O + NO3	→	BTOL4OH1O	BTOL4OH2O + NO3	→	BTOL4OH1O
B2-083		BTOL4OH2O + NO	→	BTOL4OH1O	BTOL4OH2O + NO	→	BTOL4OH1O
B2-084		BTOL4OH1O	→	0.250 AD4001 + 0.250 DK3000 + 0.250 AD5000 + 0.250 AD2000 + 0.250 AU5000 + 0.250 AA2000 + 0.250 AK5000 + 0.250 DD2000	BTOL4OH1O	→	0.250 AD4001 + 0.250 DK3000 + 0.250 AD5000 + 0.250 AD2000 + 0.250 AU5000 + 0.250 AA2000 + 0.250 AK5000 + 0.250 DD2000
B2-085		BTOL4OHOOH	→	BTOL4OH1O	BTOL4OHOOH	→	BTOL4OH1O
B2-086		BTOL4OHOOH + HO	→	BTOL4OH2O	BTOL4OHOOH + HO	→	BTOL4OH2O
B2-087		BTOL5OH2O + HO2	→	0.65 BTOL5OH1O + 0.35 BTOL5OHOOH	BTOL5OH2O + HO2	→	0.65 BTOL5OH1O + 0.35 BTOL5OHOOH
B2-088		BTOL5OH2O + NO3	→	BTOL5OH1O	BTOL5OH2O + NO3	→	BTOL5OH1O
B2-089		BTOL5OH2O + NO	→	BTOL5OH1O	BTOL5OH2O + NO	→	BTOL5OH1O

reaction ID	MG			MG-Cr			MG-Cr-Al		
B2-090				BTOL5OH1O	→	0.250 AD5000 + 0.250 AA2000 + 0.250 AA4000 + 0.250 DK3000 + 0.250 AD4001 + 0.250 AK3000 + 0.250 AK5000 + 0.250 AD2000	BTOL5OH1O	→	0.250 AD5000 + 0.250 AA2000 + 0.250 AA4000 + 0.250 DK3000 + 0.250 AD4001 + 0.250 AK3000 + 0.250 AK5000 + 0.250 AD2000
B2-091				BTOL5OHOOH	→	BTOL5OH1O	BTOL5OHOOH	→	BTOL5OH1O
B2-092				BTOL5OHOOH + HO	→	BTOL5OH2O	BTOL5OHOOH + HO	→	BTOL5OH2O
B3-004							AR0086	→	radHOM7O
B3-005							radHOM7O	→	radHOM9O
B3-006							radHOM7O + NO	→	0.80 HOM1O + 0.20 HOM1ONO2
B3-007							radHOM7O + HO2	→	HOM1OOH
B3-008							radHOM9O + NO	→	0.80 HOM2O + 0.20 HOM2ONO2
B3-009							radHOM9O + HO2	→	HOM2OOH
B3-010	AR0092	→	0.60 DD2000 + 0.40 DK3000 + 0.20 UD5000 + 0.20 UD5001 + 0.20 FURON + 0.20 MFUR + 0.20 UD4000	AR0092	→	0.60 DD2000 + 0.40 DK3000 + 0.20 UD5000 + 0.20 UD5001 + 0.20 FURON + 0.20 MFUR + 0.20 UD4000	AR0092	→	0.15 UD5001 + 0.15 DD2000 + 0.15 UD5000 + 0.15 DD2000 + 0.05 MFUR + 0.05 DD2000 + 0.20 UD4000 + 0.20 DK3000 + 0.30 FURR5 + 0.30 CH2O + 0.15 FURR3 + 0.15 D02000
B3-011	FURR5 + HO	→	FUROH	FURR5 + HO	→	FUROH	FURR5 + HO	→	FUROH
B3-019	MFUR + NO3	→	AR0121	MFUR + NO3	→	AR0121	MFUR + NO3	→	AR0121
B3-020	MFUR + O3	→	AR0121	MFUR + O3	→	AR0121	MFUR + O3	→	AR0121
B3-029	ED5000 + HO	→		ED5000 + HO	→		ED5000 + HO	→	radED5000
B3-030							radED5000 + NO	→	radED5002
B3-031							radED5000 + HO2	→	0.56 ED5000OOH + 0.44 radED5002
B3-032							ED5000OOH + HO	→	radED5000
B3-033							radED5002 + NO	→	3K2000 + CH2O
B3-034							radED5002 + HO2	→	ED5002OOH2
B3-035							ED5002OOH + HO	→	radED5002
B3-041	ED4001 + HO	→		ED4001 + HO	→		ED4001 + HO	→	radED4001
B3-042							radED4001 + NO	→	CH2O
B3-043							radED4001 + HO2	→	HD2000
B3-044							HD2000 + HO	→	DD2000

reaction ID	MG	MG-Cr	MG-Cr-Al
B5-001			UU7000 + HO → 0.32 3U7000 + 0.68 2U7000
B5-002			UU7000 + NO3 → 0.08 3U7000 + 0.92 2U7000
B5-003			UU7000 → 0.5 1U6000 + 0.5 3U7000
B5-004			2U7000 + NO → 1U7000
B5-005			2U7000 + NO3 → 1U7000
B5-006			1U7000 → 0.125 UD7000 + 0.500 UD6000 + 0.125 UD4000 + 0.125 DK3000 + 0.125 UD5000 + 0.125 DD2000 + 0.125 UD5001 + 0.125 A02000
B5-007			3U7000 + NO → 1U6000
B5-008			3U7000 + NO3 → 1U6000
B5-009			UD7000 + HO → 2D7000
B5-010			AU7000 + HO → 2D7000
B5-011			2D7000 + NO → 1D7000
B5-012			2D7000 + HO2 → AU70002
B5-013			2D7000 + NO3 → 1D7000
B5-014			1D7000 → 0.05 AU5002 + 0.05 AD2000 + 0.35 AU4000 + 0.35 AK3000 + 0.35 DK4000 + 0.35 DK3000 + 0.25 DD3000 + 0.25 DK4001
B5-015			AU6000 + HO → 2D6000
B5-016			UD6000 + HO → 2D6001
B5-017			2D6000 + NO → 1D6000
B5-018			2D6000 + HO2 → DK4000 + AD20002
B5-019			2D6000 + NO3 → 1D6000
B5-020			2D6001 + NO → 1D6001
B5-021			2D6001 + HO2 → AU60002
B5-022			2D6001 + NO3 → 1D6001
B5-023			1D6000 → AD2000 + DK4000
B5-024			1D6001 → DK3000 + DD3000
B6-011	UD5000 + HO → 0.54 3U5002 + 0.23 2D5003	UD5000 + HO → 0.54 3U5002 + 0.23 2D5003	UD5000 + HO → 0.54 3U5002 + 0.23 FURR6 + 0.23 2D5003

References

Bosque, R.; Sales, J. J. Chem. Inf. Comput. Sci. 2002, 42 (5), 1154−1163.

De Haan, D. O., Jimenez, N. G., de Loera, A., Cazaunau, M., Gratien, A., Pangui, E., and Doussin, J.-F.: Methylglyoxal Uptake Coefficients on Aqueous Aerosol Surfaces, J. Phys. Chem. A, 122, 4854–4860, https://doi.org/10.1021/acs.jpca.8b00533, 2018.

Eichler, P., Müller, M., D'Anna, B., and Wisthaler, A.: A novel inlet system for online chemical analysis of semi-volatile submicron particulate matter, Atmos. Meas. Tech., 8, 1353–1360, https://doi.org/10.5194/AMT-8-1353-2015, 2015.

Ellis, A. M.; Mayhew, C. A. Proton Transfer Reaction Mass Spectrometry; John Wiley & Sons, Ltd: Hoboken, NJ, 2014; pp 25−48.

Gioumousis, G.; Stevenson, D. P. J. Chem. Phys. 1958, 29, 294−299.

Hu, J., Chen, Z., Qin, X., and Dong, P.: Reversible and irreversible gas-particle partitioning of dicarbonyl compounds observed in the real atmosphere, Atmos. Chem. Phys, 22, 6971–6987, https://doi.org/10.5194/acp-22-6971-2022, 2022.

Huang, Y., Zhao, R., Charan, S. M., Kenseth, C. M., Zhang, X., and Seinfeld, J. H.: Unified Theory of Vapor-Wall Mass Transport in Teflon-Walled Environmental Chambers, Environ. Sci. Technol., 52, 2134–2142, https://doi.org/10.1021/acs.est.7b05575, 2018.

Krechmer, J. E., Pagonis, D., Ziemann, P. J., and Jimenez, J. L.: Quantification of Gas-Wall Partitioning in Teflon Environmental Chambers Using Rapid Bursts of Low-Volatility Oxidized Species Generated in Situ, Environ. Sci. Technol., 50, 5757–5765, https://doi.org/10.1021/acs.est.6b00606, 2016.

Langevin, P. J. Chim. Phys. Phys. Chim. Biol. 1903, 28, 433−530.

Müller, M., Mikoviny, T., Jud, W., D'Anna, B., and Wisthaler, A.: A new software tool for the analysis of high resolution PTR-TOF mass spectra, Chemom. Intell. Lab. Syst., 127, 158–165, https://doi.org/10.1016/J.CHEMOLAB.2013.06.011, 2013.

Su, T.; Chesnavich, W. J. J. Chem. Phys. 1982, 76, 5183−5185.

Zhang, X., Schwantes, R. H., McVay, R. C., Lignell, H., Coggon, M. M., Flagan, R. C., and Seinfeld, J. H.: Vapor wall deposition in Teflon chambers, Atmos. Chem. Phys., 15, 4197–4214, https://doi.org/10.5194/ACP-15-4197-2015, 2015.