Cloud Processing of Secondary Organic Aerosol from Isoprene and Methacrolein Photooxidation

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S1   Experimental section

S1.1   Details of Isoprene experiments

Table S1. Type of experiments, experimental conditions, SOA yields, generated clouds and instrumental analysis (mass spectrometry) of SOA for isoprene experiments.

Experiments	$[VOC]_0^a$ ppb	$[HONO]_0$ ppb	$[NO]_0$ ppb	$[NO_2]_0$ ppb	$[O_3]_{max}$ ppb	$\Delta M_0^{b,c}$ µg/m³	T °C	RH %	N clouds	MS measurements[d] AMS	GC-MS
					Blanks						
B-120115	0	137	195	104	2	<0.3	19.6	0	-	N	Y
					Isoprene - Control experiment						
IC-040315	755	223	165	93	306	4.9	20.2	0.5	-	N	Y
					Isoprene - Diphasic experiments						
ID-300113[e]	817	161	95	71		<0.1		4-3	2	Y	Y
ID-010213[e]	800	133	103	49		<0.1		2-1	2	Y	Y
					Isoprene - Triphasic experiments						
IT-090113[e,f]	375	2.2	44	0	94	4.3	21.9	0	2	Y	Y
IT-160113[e,f]	846	15	143	27	122	<0.1			1	Y	Y
IT-280113[e,f]	833	125	88	45	201	2.8		3-2	2	Y	Y
IT-160614	850	161	91	154	212	5.5	23.1	9	2	Y	Y

[a] Measurement uncertainty is 15 ppb. [b] SOA concentration with effective density of 1.4 g/cm³. [c] Measurement uncertainty is 0.1 µg/m³. [d] Y=yes, N=no. [e] (Brégonzio-Rozier et al., 2016). [f] (Brégonzio-Rozier et al., 2015)

S1.2   Principal Component analysis

Principal component analysis (PCA) was applied to time-series of the concentrations of organics, nitrate and ammonium to extract the underlying factors, or latent variables, contributing to the timeseries of organics in high humidity conditions (i.e. production of SOA *vs.* evaporative losses). The latent variables, hereafter called principal components, are orthogonal linear combinations of the original variables in which the first component (PC 1) explains most of the variance of the dataset and the second component (PC 2) explains most of the residual variance (Wold et al., 1987). PCA was performed using the package "R commander" in R 3.2.5 on three variables (concentrations of organics, nitrate and ammonium measured with the HR-ToF-AMS) and 284 cases for experiment MT-180113, 249 cases for experiment MT-210113 and 251 cases for experiment MT-230113. For all three experiments the first two components were selected on the basis of the scree plots (not shown), explaining 98-99% of the variance of the datasets (66-72% by PC 1).

Principal components were used to disaggregate production of organic aerosol during clouds (explained by PC 1) from the production of organic aerosol in dry conditions and evaporative losses (both explained by PC 2). In order to do so, the weighted (by multiplying for the PC loadings for organics) sum of scores of the three principal components (explaining 100% of variance) was scaled to match the total amount of organics measured by the HR-ToF-AMS for each case using a linear regression (r^2=1). The PC 1 corrected scores were then used to estimate the production of organic aerosol during cloud events corrected for evaporative losses (PC 2).

S1.3   Aqueous phase experiments

Aqueous phase experiments were performed using a photoreactor (detailed in Renard et al. (2013)). The reactor was a 450 cm^3 Pyrex thermostated photoreactor, equipped with a 1000 W Xenon arc lamp (LOTOriel, LSH 601) and a glass filter (ASTM Air Mass 1.5), simulating the solar irradiation in the UV-visible wavelengths at ground level. All experiments were performed at 25 °C, and started with irradiation of UHQ water (18.2 MΩ cm, Millipore). Then H_2O_2 (Acros, 30%, non-stabilized) was introduced, and after 10 min of H_2O_2 photolysis, methacrolein (Sigma Aldrich, 95%) was introduced at time 0. The experiments were carried out with methacrolein initial concentrations of 20 mM (thus corresponding to 960 mgC/L). The 50 cm^3 gas-phase head space of the photoreactor was opened to ambient air for a few seconds during each sampling. We verified in control experiments that this procedure induced insignificant losses of methacrolein (MACR) from the solution. Due to the very fast reactivity of MACR added to the fact that the photoreactor was closed most of the time, this procedure induced a significant decrease in the dissolved O_2 concentrations, down to 0.5 mg/L after 30 minutes of reaction, in a similar way as in experiments performed with methylvinyl ketone (Renard et al., 2013). The initial H_2O_2 concentrations were chosen in order to obtain a ratio $[H_2O_2]_0 / [MACR]_0 = 20$, in order to favor ·OH reaction with MACR rather than with H_2O_2 by more than 80%. Under these conditions, we estimate that the ·OH concentrations were approximately $10^{-14} - 10^{-13}$ M, in the range of the estimated values for fog droplets to wet aerosol conditions (Arakaki et al., 2013; Ervens et al., 2014; Herrmann et al., 2015, 2010).

S2   Results

S2.1   Evaporative losses at high RH and SOA production during cloud events

Table S2. Increase of concentration of VOCs and decrease of aerosol mass upon increase of RH from <5% to 80-90% before cloud formation.

Experiments	Δ[VOCs][a]	[SOA][b] loss	[SOA][b] loss
	μg/m^3	μg/m^3	%
MT-180113	494	-18.2	-31%
MT-210113	454	-21.2	-32%
MT-230113	381	-6.7	-25%

[a] Measurement uncertainty ~50%. [b] SMPS measurements.

Table S3. Decrease of gas phase concentrations of VOCs and SOA production during clouds events measured with AMS and extrapolated with PCA by correcting for evaporative losses.

Experiments Events	Δ[VOCs][a]	[NO$_3^-$]$_{max}$	[NH$_4^+$]$_{max}$	[Org.]$_{max}$[b] measured	Δ[SOA] measured	SOA mass yields (measured)	[Org.]$_{max}$ (PCA)	Δ[SOA] (PCA)	SOA mass yields (PCA)
	μg/m^3	μg/m^3	μg/m^3	μg/m^3	μg/m^3		μg/m^3	μg/m^3	
MT-180113									
1st cloud	145	1.34±0.03	0.41±0.01	4.3±0.5	6.0±0.5	3.1±0.3·10^{-3}	12±2	14±2	6.7±0.9·10^{-3}
2nd cloud	12	0.59±0.03	0.16±0.01	1.8±0.2	2.5±0.3	1.3±0.1·10^{-3}	5±2	6±2	2.9±0.9·10^{-3}
MT-210113									
1st cloud	265	0.44±0.03	0.21±0.01	25±32	25±33	12±16·10^{-3}	44±12	45±12	22±6·10^{-3}
2nd cloud	91	0.24±0.03	0.16±0.01	33±26	33±26	16±13·10^{-3}	14±6	14±7	6.9±3.2·10^{-3}
MT-230113									
1st cloud	183	0.14±0.03	0.04±0.01	2.6±3.3	2.8±3.3	2.9±3.4·10^{-3}	16±4	16±4	16±4·10^{-3}
2nd cloud	87	0.22±0.03	0.07±0.01	1.9±0.4	2.2±0.5	2.3±0.5·10^{-3}	25±3	26±3	26±4·10^{-3}

[a] Measurement uncertainty ~50%. [b] calculated by log-normal fitting of the 2nd mode produced during clouds.

S2.2 Repartitioning of water soluble VOCs into cloud droplets
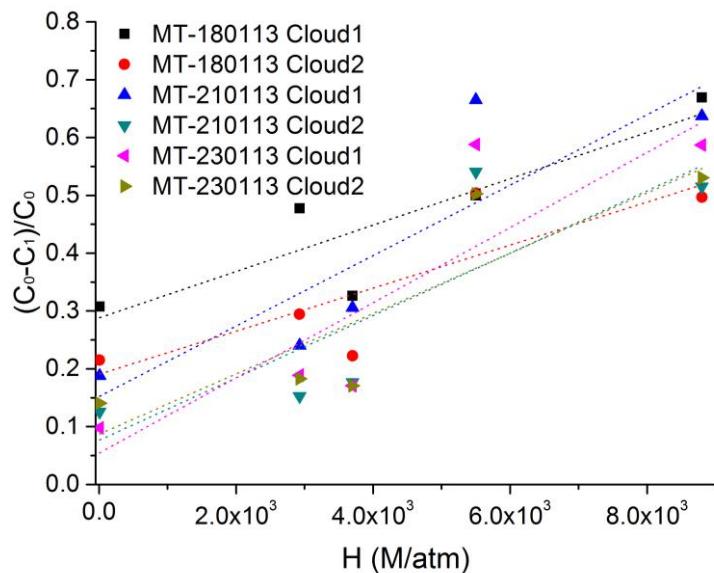

Figure S1. Linear relation between the relative decrease in gas phase concentrations of water soluble VOCs during cloud events and their Henry's law constant (H) for acrolein (Sander, 2015)**, hydroxyacetone** (Ito et al., 2007)**, methylglyoxal** (Ito et al., 2007)**, formic acid** (Sander, 2015) **and acetic acid** (Sander, 2015)**. Dotted lines show linear regressions (r^2 0.61-0.71).**

S2.3 Ratios NO^+/NO_2^+ and NH_4^+/NO_3^- from HR-ToF-AMS measurements in methacrolein and isoprene experiments, inorganic salts and organonitrogen compounds

Table S4. Measured NO^+/NO_2^+ (mass ratio) and NH_4^+/NO_3^- (molar ratio) in methacrolein experiments during cloud events and corresponding values for standard compounds.

Experiments	Events	NO^+/NO_2^+ (clouds)	NH_4^+/NO_3^- (molar ratio)	Description of experiment	References
MT-180113	1st cloud	2.36±0.12	1.07±0.02	methacrolein triphasic	This study
	2nd cloud	2.58±0.32	1.08±0.08		
MT-210113	1st cloud	3.34±0.33	1.78±0.13	methacrolein triphasic	This study
	2nd cloud	3.51±0.49	2.55±0.41		
MT-230113	1st cloud	2.67±0.30	1.15±0.18	methacrolein triphasic	This study
	2nd cloud	2.66±0.22	1.11±0.08		
MT-130614	1st cloud	2.68±0.17	1.03±0.60	methacrolein triphasic (60% RH)	This study
	2nd cloud	2.95±0.35	0.95±0.16		
IT-280113	1st cloud	2.02±0.10	1.01±0.02	isoprene triphasic	(Brégonzio-Rozier et al., 2016)
	2nd cloud	1.99±0.06	1.02±0.03		
ID-300113	1st cloud	2.01±0.12	1.02±0.04	isoprene diphasic	(Brégonzio-Rozier et al., 2016)
	2nd cloud	1.96±0.13	1.00±0.02		
NH_4NO_3		2.44	1.00	ammonium nitrate standard	This study
		2.4			(Bruns et al., 2010)
$NaNO_3$		29		sodium nitrate standard	(Rollins et al., 2010)
		80			(Bruns et al., 2010)
$NaNO_2$		73±6		sodium nitrite standard	This study
$C_4H_9NO_4$		1.83		1-hydroxy-butane-2-nitrate	(Rollins et al., 2010)
$C_{10}H_{17}NO_4$		0.99		3-hydroxy-pinene-2-nitrate	(Rollins et al., 2010)
$C_{10}H_{17}NO_4$		5.30		2-hydroxy-limonene-1-nitrate	(Rollins et al., 2010)
$C_{15}H_{25}NO_4$		4.48		3-hydroxy-caryophyllene-4-nitrate	(Rollins et al., 2010)
$C_6H_9NO_6$		10-15		isosorbide 5-mononitrate	(Bruns et al., 2010)
$C_3H_4NO_3$		5		nitroxyacetone standard	This study
$C_5H_{11}NO_2$		5.5		isopentylnitrite standard	This study

S2.4 Results from MonomerHunter of high-resolution data

Table S5. Monomers extracted using "MonomerHunter" from CHO compounds detected in HRMS analysis of SOA from the photooxidation of methacrolein in control, triphasic, triphasic at 60% RH and aqueous phase experiments. Monomers selected for Figure 8 are highlighted in bold green.

Monomers	N pairs control experiments	N pairs triphasic experiments	N pairs triphasic experiments at 60% RH	N pairs aqueous experiments	Tentative assignment	References
CH$_2$	218	109	761	791	methyl	
CH$_2$O	149	68	657	777	formaldehyde	
C$_4$H$_6$O$_3$	316	107	635	579	2-methylglyceric acid (–H$_2$O)	(Nguyen et al., 2011, 2010)
O	125	52	627	790	oxygen	
C$_2$H$_4$O	121	102	618	734	acetaldehyde/ethylene glycol	(Nguyen et al., 2011)
C$_2$H$_2$O	156	88	589	731	glycolaldehyde	(Nguyen et al., 2011)
C$_2$H$_4$O$_2$	157	80	575	674	glycolaldehyde	(Nguyen et al., 2011)
CO	109	80	569	709	carbon monoxide	
C$_3$H$_4$O	117	78	538	708	hydroxyacetone (–H$_2$O)	(Nguyen et al., 2011)
CH$_2$O$_2$	124	60	546	685	formic acid	(Nguyen et al., 2010)
C$_3$H$_4$O$_2$	124	66	547	659	lactic acid/methylglyoxal, acrylic acid/methylglyoxal	(Nguyen et al., 2011, 2010)
C$_3$H$_4$O$_3$	182	68	564	559	pyruvic acid/hydrolyzed methylglyoxal	(Nguyen et al., 2011, 2010)
C$_3$H$_6$O$_2$	98	71	529	644	hydroxyacetone	(Nguyen et al., 2011)
C$_3$H$_6$O	73	46	538	677	acetone	
C$_2$H$_2$O$_2$	109	49	533	641	hydroxyacetic acid (–H$_2$O)	(Nguyen et al., 2011)
C$_5$H$_8$O$_3$	160	80	525	567	2-hydroxy-2-methylbutanedial	(Nguyen et al., 2011)
C$_4$H$_6$O$_2$	101	50	508	658	methacrylic acid/2-methylglyceraldehyde (–H$_2$O)	(Nguyen et al., 2011, 2010)
H$_2$O	81	59	444	718	water	
C$_4$H$_6$O	68	43	479	687	methacrolein	
O$_2$	80	33	523	641	oxygen	
CO$_2$	71	34	504	598	carbon dioxide	
C$_2$H$_2$O$_3$	118	32	523	522		
C$_4$H$_8$O$_2$	60	62	455	597		
C$_5$H$_8$O$_2$	67	39	436	608		
C$_5$H$_8$O$_4$	132	48	472	486		
C$_3$H$_6$O$_3$	96	41	404	573		
C$_4$H$_8$O	42	23	446	582		
C$_2$H$_4$O$_3$	82	28	393	581	glycolic acid	(Nguyen et al., 2010)
C$_4$H$_6$O$_4$	105	32	475	471		
C$_5$H$_8$O	37	21	409	591	2-methyl-2-butenal	
C$_4$H$_8$O$_3$	75	36	378	562	2-MG aldehyde	(Nguyen et al., 2011)
C$_4$H$_8$O$_4$	70	37	330	491	2-methylglyceric acid	(Nguyen et al., 2011, 2010)

Table S6. Monomers extracted using "MonomerHunter" from CHNO compounds detected in HRMS analysis of SOA from the photooxidation of methacrolein in control, triphasic and triphasic at 60% RH experiments. Monomers selected for Figure 8 are highlighted in bold green, N-containing monomers are highlighted in bold red.

Monomers	N pairs control experiments	N pairs triphasic experiments	N pairs triphasic experiments at 60% RH	Tentative assignment	References
$C_4H_6O_3$	205	205	500	2-methylglyceric acid acetic anhydride	(Nguyen et al., 2011, 2010)
$C_5H_8O_3$	375	124	306	2-hydroxy-2-methylbutanedial	(Nguyen et al., 2011)
$C_2H_4O_2$	301		337	glycolaldehyde	(Nguyen et al., 2011)
CH_2	202	139	292	methyl	
CH_2O	304		284	formaldehyde	
$C_3H_4O_2$	266	29	246	lactic acid/methylglyoxal, acrylic acid/methylglyoxal	(Nguyen et al., 2011, 2010)
$C_2H_2O_3$	217	45	245		
CO	141	74	250	carbon monoxide	
CH_2O_2	194		262	formic acid	(Nguyen et al., 2010)
C_3H_4O	170		248	hydroxyacetone (–H_2O)	(Nguyen et al., 2011)
$C_3H_4O_3$		93	313	pyruvic acid/hydrolyzed methylglyoxal	(Nguyen et al., 2011, 2010)
$C_5H_8O_5$	149	52	196		
$C_3H_6O_2$	142		252	hydroxyacetone	(Nguyen et al., 2011)
C_2H_4O	131		258	acetaldehyde/ethylene glycol	(Nguyen et al., 2011)
$C_4H_6O_4$	168	12	186		
C_2H_2O	78	115	165	glycolaldehyde	(Nguyen et al., 2011)
$C_4H_6O_2$	147	18	192	methacrylic acid/2-methylglyceraldehyde (–H_2O)	(Nguyen et al., 2011, 2010)
$C_5H_6O_4$	105	50	182		
O		28	263	oxygen	
CO_3	110		199		
$C_4H_6O_5$	95	28	168		
$C_3H_6O_4$	85	29	166	glyceric acid	
$C_5H_8O_4$	80		199		
$C_3H_6O_3$	131		143		
H_2O	87		185	water	
$C_5H_6O_3$	118		154		
$C_2H_4O_3$	122	12	135	glycolic acid	(Nguyen et al., 2010)
$C_5H_8O_2$	67	11	176		
$C_4H_4O_3$	101		149		
$C_5H_6O_5$	95		150		
$C_4H_4O_2$	78		165		
$C_5H_{10}O_4$	54	28	146		
$C_5H_6O_6$	89		137		
$C_3H_4O_5$	68		152		
C_4H_6O		34	186	methacrolein	
$C_4H_8O_4$	68		147	2-methylglyceric acid	(Nguyen et al., 2011, 2010)

$C_4H_8O_3$	88		124	2-MG aldehyde	(Nguyen et al., 2011)
$C_3H_4O_4$	50		161		
C_5H_8O	47	13	145	2-methyl-2-butenal	
$C_2H_2O_2$			200	hydroxyacetic acid (–H_2O)	(Nguyen et al., 2011)
$C_5H_6O_2$	68		130		
$CHNO_2$	112		75		
$C_4H_4O_6$	57		128		
C_3H_6O			183	acetone	
$C_5H_7NO_5$	99	23	55		
$C_5H_8O_6$	75		97		
$C_4H_8O_2$			171		
$C_5H_{10}O_3$	44		127	2,4-dihydroxy-2-methylbutanal	

S2.5 Oligomer series of CHNO compounds in smog chamber experiments
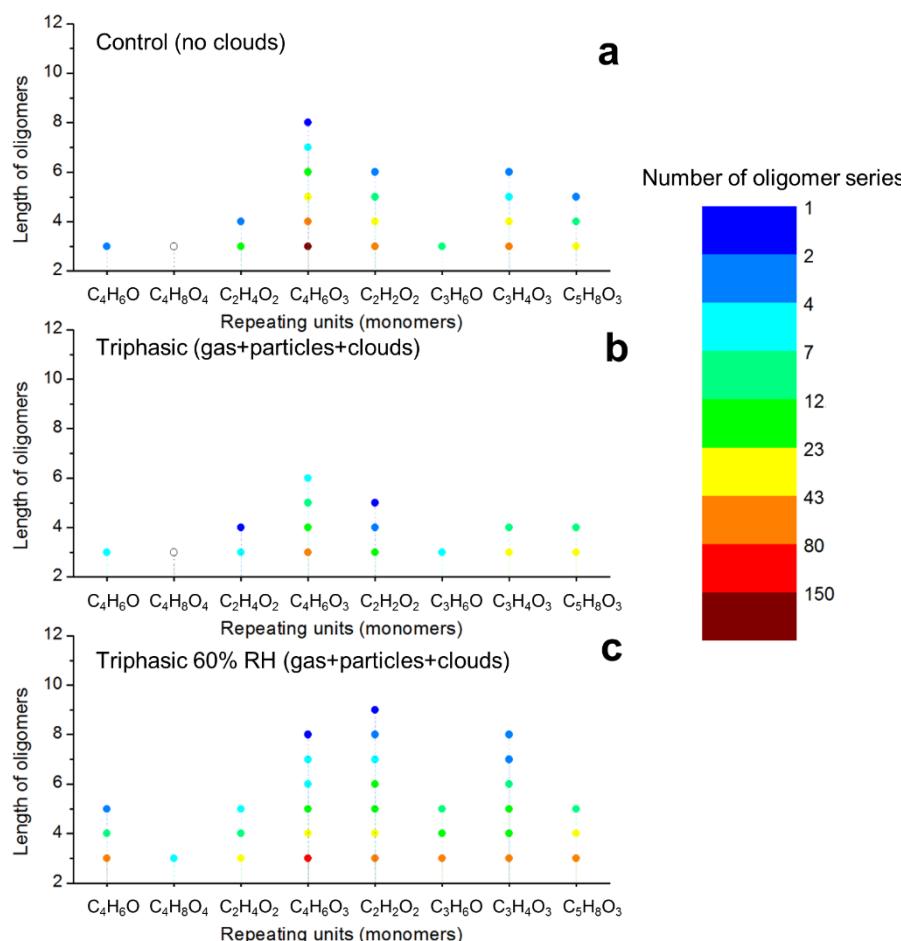
Figure S2. N-containing trimers and longer oligomers detected in methacrolein photooxidation experiments in control conditions without clouds (a), in triphasic conditions with two cloud events (b) and in triphasic conditions starting at 60% RH with two cloud events (c). Molecular formulas of the repeating units can be associated with (from left to right) methacrolein (C_4H_6O), 2-methylglyceric acid ($C_4H_8O_4$), glycolaldehyde ($C_2H_4O_2$), methylglyceric acid ($C_4H_6O_3$ because of H_2O loss), hydroxyacetic acid ($C_2H_2O_2$), acetone (C_3H_6O), pyruvic acid/hydrolyzed methylglyoxal ($C_3H_4O_3$) and 2-hydroxy-2-methylbutanedial ($C_5H_8O_3$).

S2.6 Oligomer series in aqueous phase experiments
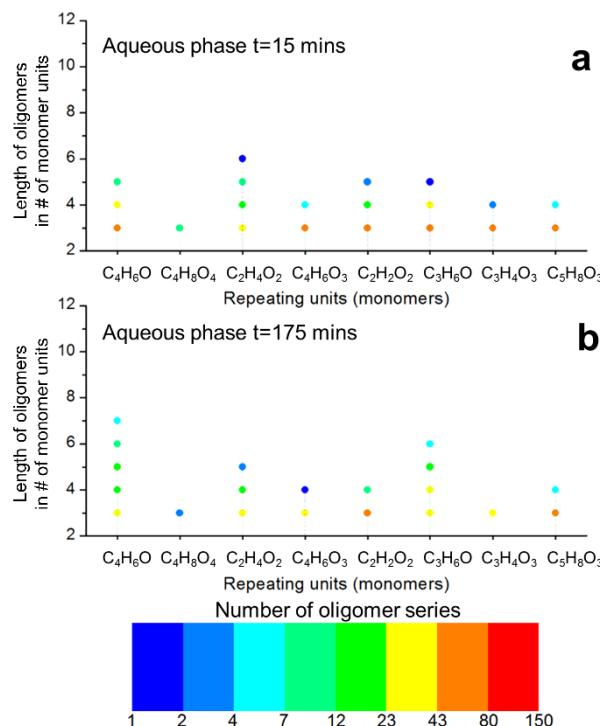

Figure S3. Trimers and longer oligomers (CHO compounds only) detected in methacrolein photooxidation experiments in NO$_x$ free conditions in the aqueous phase with 15 min reaction time (a) and 175 min reaction time (b). Molecular formulas of the repeating units can be associated with (from left to right) methacrolein (C$_4$H$_6$O), 2-methylglyceric acid (C$_4$H$_8$O$_4$), glycolaldehyde (C$_2$H$_4$O$_2$), methylglyceric acid (C$_4$H$_6$O$_3$ because of H$_2$O loss), hydroxyacetic acid (C$_2$H$_2$O$_2$), acetone (C$_3$H$_6$O), pyruvic acid/hydrolyzed methylglyoxal (C$_3$H$_4$O$_3$) and 2-hydroxy-2-methylbutanedial (C$_5$H$_8$O$_3$).

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