Supplementary information for manuscript

Secondary organic aerosol formed by EURO 5 gasoline vehicle emissions: Chemical composition and gas-to-particle phase partitioning

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Quantification of the PTR-ToF-MS signal

Ionization of organic compounds (except some small hydrocarbons) by PTR-MS occurs with a collisional rate, which can be accurately predicted by ion−molecule collision theories (Ellis et al. 2013). The instrumental response factors for pure hydrocarbons were estimated using the Langevin−Gioumousis−Stevenson theory (Langevin, 1903; Gioumousis and Stevenson 1958). The instrumental sensitivities of heteroatom-containing hydrocarbons were calculated based on the Su and Chesnavich, (1982) rate theory. Thus the instrumental response factor can be estimated using the weight, the isotropic molecular polarizability, and the dipole moment of an analyte molecule. For the molecular weight we used the observed *m/z* −1 (accounting for the added proton) assuming that the molecule does not fragment upon protonation. Isotropic molecular polarizabilities were determined from the analyte ions' elemental composition using the parametrization proposed by Bosque and Sales, (2002). For the dipole moment a constant value of 2.75 D was used for all heteroatom-containing analyte ions. This value corresponds to an average value of typical dipole moments of oxygenated hydrocarbons (1−4.5 D), resulting in a a maximum quantification uncertainty of ±40%. For example methylglyoxal, which has a low dipole moment ($\mu D = 0.992$ D) has an uncertainty of ±30%. Signals with unidentified elemental composition were quantified using a proton reaction rate constant of 2×10^{-9} cm^3 s^{-1}. The total SOA mass concentration was calculated by adding the mass concentrations of all detected *m/z* peaks.

Table S1: Number of the total m/z's detected, number of the detected m/z's with contribution higher than 0.14% to the total concentration (in ppb) and the corresponding fraction explained by these m/z's for fresh VOC, secondary VOC and SOA.

	Exp #1	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
Fresh VOC					
Number of total detected m/z's	61	59	59	67	103
Number of detected m/z's with contribution >0.14% to the total concentration	49	47	48	53	75
Fraction explained by the m/z's with contribution >0.14%	0.99	0.99	0.99	0.98	0.96
SVOC					
Number of total detected m/z's	163	95	92	112	108
Number of detected m/z's with contribution >0.14% to the total concentration	95	63	62	72	69
Fraction explained by the m/z's with contribution >0.14%	0.93	0.97	0.97	0.96	0.96
SOA					
Number of total detected m/z's	237	169	190	184	253
Number of detected m/z's with contribution >0.14% to the total concentration	156	110	124	113	179
Fraction explained by the m/z's with contribution >0.14%	0.92	0.94	0.93	0.93	0.95

Table S2: List of the measured accurate *m/z's* and elemental composition $C_xH_yN_zO_w^+$ of the most significant detected ions with concentration higher than 0.14% of the total detected ion concentration of the fresh emissions in the chamber (before any dilution in the chamber) during cold urban (experiments #1, 2 and 3), hot urban (experiment #4) and motorway (experiment # 5) Artemis cycles. These ions explained 85-99% of the measured concentration.

		Concentration (ppb)				
m/z	**Molecular type**	**Exp #1**	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
28.03	$(C_2H_3)H^+$	22.8	28.7	30.3	0.9	1.0
29.04	$(C_2H_4)H^+$	8.4	7.4	11.5	-	-
31.02	$(CH_2O)H^+$	18.2	25.1	15.1	-	-
33.03	$(CH_3OH)H^+$	28.5	16.4	19.2	0.6	1.0
41.04	$(C_3H_4)H^+$	41.2	76.5	57.7	1.1	1.4
42.03	$(C_2H_3N)H^+$	-	-	8.3	1.3	1.4
42.05	$(C_3H_5)H^+$	15.0	23.1	20.5	1.1	1.1
43.05	$(C_3H_6)H^+$	188.9	299.4	274.7	6.2	4.5
44.06	$([13C]C_2H_6)H^+$	6.2	9.8	9.2	0.3	0.4
45.03	$(C_2H_4O)H^+$	53.1	69.1	71.1	0.9	2.1
47.05	$(C_2H_6O)H^+$	97.8	100.2	106.5	0.7	1.2
56.06	$(C_4H_7)H^+$	20.1	26.7	25.0	1.5	0.8
57.03	$(C_3H_4O)H^+$	9.3	10.9	9.8	0.2	0.3
57.07	$(C_4H_8)H^+$	362.8	493.6	457.1	14.6	8.0
58.07	$([13C]C_3H_8)H^+$	16.3	21.9	20.2	0.6	0.4
59.05	$(C_3H_6O)H^+$	13.9	14.7	26.0	0.9	1.7
67.05	$(C_5H_6)H^+$	10.7	16.4	13.2	-	-
69.07	$(C_5H_8)H^+$	24.1	39.2	31.5	0.3	0.8
70.07	$([13C]C_4H_8)H^+$	11.7	14.5	13.9	0.9	0.3
71.05	$(C_4H_6O)H^+$	6.9	6.5	6.4	-	0.3
71.09	$(C_5H_{10})H^+$	134.8	192.1	166.6	5.1	3.0
72.09	$([13C]C_4H_{10})H^+$	7.9	10.6	9.2	0.3	0.2
78.05	$(C_6H_5)H^+$	10.8	13.9	15.6	1.6	0.4
79.05	$(C_6H_6)H^+$	155.6	212.4	245.8	15.7	5.8
80.06	$([13C]C_5H_6)H^+$	11.9	15.1	17.0	1.1	0.5
81.07	$(C_6H_8)H^+$	5.2	8.0	7.6	-	0.2
83.09	$(C_6H_{10})H^+$	14.8	19.4	17.0	0.3	0.4
85.10	$(C_6H_{12})H^+$	71.6	87.8	81.9	2.3	1.7
91.05	$(C_7H_6)H^+$	13.1	14.6	14.9	0.5	0.4
92.06	$([13C]C_6H_6)H^+$	16.6	22.3	21.4	1.2	0.2
93.07	$(C_7H_8)H^+$	306.7	381.6	375.1	13.8	3.8
94.07	$([13C]C_6H_8)H^+$	25.2	29.3	28.5	1.1	0.4
97.10	$(C_7H_{12})H^+$	5.2	6.1	6.0	-	0.2
105.07	$(C_8H_8)H^+$	34.7	56.3	44.6	0.8	1.5
106.07	$([13C]C_7H_8)H^+$	34.2	42.7	41.1	1.3	0.4
107.09	$(C_8H_{10})H^+$	824.7	963.7	1029.0	19.2	8.8
108.09	$([13C]C_7H_{10})H^+$	77.7	84.0	86.3	1.7	0.8

111.12	$(C_8H_{14})H^+$	5.4	-	6.2	0.2	0.3
117.07	$(C_9H_8)H^+$	5.2	10.8	8.9	0.2	0.4
119.09	$(C_9H_{10})H^+$	34.1	47.8	36.5	0.7	2.1
120.09	$([13C]C_8H_{10})H^+$	21.9	26.0	24.2	0.7	0.6
121.10	$(C_9H_{12})H^+$	435.9	537.4	552.5	9.7	9.9
122.11	$([13C]C_8H_{12})H^+$	46.9	52.8	53.0	1.0	1.0
129.07	$(C_{10}H_8)H^+$	-	10.1	6.6	1.4	2.0
133.10	$(C_{10}H_{12})H^+$	4.8	9.9	6.7	0.4	0.8
135.12	$(C_{10}H_{14})H^+$	38.4	59.1	50.1	2.3	3.0
136.12	$([13C]C_9H_{14})H^+$	-	6.2	-	0.2	0.3
Fraction of the above compounds to the total fresh VOC		**0.95**	**0.98**	**0.99**	**0.90**	**0.85**

Table S3: List of the measured accurate *m/z's* and elemental composition $C_xH_yN_zO_w^+$ of the most significant detected ions with concentration higher than 0.14% of the total detected ion concentration of the secondary gas phase products produced from cold urban (experiments #1, 2 and 3), hot urban (experiment #4) and motorway (experiment # 5) Artemis cycles emissions. These ions represented 89-97% of the measured concentration.

		Concentration (ppb)				
m/z	**Molecular type**	**Exp #1**	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
31.02	$(CH_2O)H^+$	62.0	17.9	16.9	2.2	1.1
33.03	$(CH_3OH)H^+$	5.9	1.7	8.7	1.8	1.8
43.02	$(C_2H_2O)H^+$	85.1	16.4	54.9	11.1	5.4
45.03	$(C_2H_4O)H^+$	203.0	72.7	78.9	13.1	5.0
46.03	**$(CH_3NO)H^+$**	12.4	-	6.2	2.5	1.0
47.01	$(CH_2O_2)H^+$	17.7	2.3	60.5	4.9	-
57.03	$(C_3H_4O)H^+$	19.8	6.7	7.6	1.3	0.8
59.01	$(C_2H_2O_2)H^+$	3.5	-	-	-	0.1
59.05	$(C_3H_6O)H^+$	185.3	66.6	74.3	18.4	7.7
60.04	**$(C_2H_5NO)H^+$**	3.9	-	2.5	1.1	-
61.03	$(C_2H_4O_2)H^+$	100.3	15.1	88.2	21.0	10.2
71.01	$(C_3H_2O_2)H^+$	2.8	0.2	0.4	0.2	0.1
71.05	$(C_4H_6O)H^+$	12.7	4.1	2.5	0.8	0.6
73.03	$(C_3H_4O_2)H^+$	94.3	28.1	36.0	4.2	1.7
73.06	$(C_4H_8O)H^+$	42.1	13.4	13.7	3.1	1.1
74.03	$([13C]C_2H_4O_2)H^+$	2.7	0.5	1.2	0.5	0.4
75.04	$(C_3H_6O_2)H^+$	18.5	3.7	12.8	2.0	1.5
77.02	$(C_2H_4O_3)H^+$	10.0	1.0	21.5	1.2	0.5
83.01	$(C_4H_2O_2)H^+$	7.1	0.7	2.8	0.8	0.6
83.05	$(C_5H_6O)H^+$	2.7	0.6	-	-	-
85.03	$(C_4H_4O_2)H^+$	8.5	1.2	1.4	0.4	0.2
85.06	$(C_5H_8O)H^+$	6.5	1.8	1.9	0.6	0.3
87.04	$(C_4H_6O_2)H^+$	31.2	8.9	13.6	2.7	1.0
87.08	$(C_5H_{10}O)H^+$	16.3	5.1	5.9	1.3	0.4
89.02	$(C_3H_4O_3)H^+$	6.5	0.6	2.1	0.7	0.4
89.06	$(C_4H_8O_2)H^+$	4.4	0.7	3.1	1.1	0.7
90.02	**$(C_2H_3NO_3)H^+$**	2.9	-	1.4	0.4	0.2
95.05	$(C_6H_6O)H^+$	2.3	0.6	-	0.2	-
97.03	$(C_5H_4O_2)H^+$	8.5	0.7	2.0	0.3	0.1
98.02	**$(C_4H_3NO_2)H^+$**	2.2	-	-	0.2	0.1
99.01	$(C_4H_2O_3)H^+$	12.9	1.9	6.5	0.8	0.9
99.04	$(C_5H_6O_2)H^+$	23.9	4.9	3.6	0.7	0.3
99.08	$(C_6H_{10}O)H^+$	5.6	1.7	1.7	0.6	0.2
100.04	**$(C_4H_5NO_2)H^+$**	3.9	0.5	-	0.3	0.1
101.02	$(C_4H_4O_3)H^+$	7.1	0.7	2.8	0.8	0.6
101.06	$(C_5H_8O_2)H^+$	8.6	2.1	3.3	0.8	0.4
101.10	$(C_6H_{12}O)H^+$	5.0	1.4	1.6	0.3	0.1

103.04	$(C_4H_6O_3)H^+$	6.0	-	1.3	0.3	0.1
107.05	$(C_7H_6O)H^+$	7.4	0.6	2.0	-	-
109.03	$(C_6H_4O_2)H^+$	-	-	1.8	0.3	0.4
109.07	$(C_7H_8O)H^+$	3.1	1.3	-	-	-
111.04	$(C_6H_6O_2)H^+$	11.4	1.0	2.0	0.2	-
112.04	**$(C_5H_5NO_2)H^+$**	4.7	0.6	-	0.2	-
113.02	$(C_5H_4O_3)H^+$	25.2	3.4	8.8	1.0	0.7
113.06	$(C_6H_8O_2)H^+$	29.0	8.5	3.6	0.7	0.3
113.10	$(C_7H_{12}O)H^+$	5.1	1.3	1.2	0.6	0.1
115.04	$(C_5H_6O_3)H^+$	11.6	1.2	3.6	0.6	0.4
115.08	$(C_6H_{10}O_2)H^+$	4.1	1.2	2.1	0.6	0.2
117.02	$(C_4H_4O_4)H^+$	2.3	0.2	0.5	0.1	0.1
121.07	$(C_8H_8O)H^+$	10.9	2.7	3.8	0.2	-
123.04	$(C_7H_6O_2)H^+$	3.1	0.5	1.6	0.2	0.3
125.02	$(C_6H_4O_3)H^+$	2.3	-	1.0	0.2	0.2
125.06	$(C_7H_8O_2)H^+$	5.4	0.5	1.0	-	-
127.04	$(C_6H_6O_3)H^+$	10.3	1.2	3.1	0.4	0.3
127.08	$(C_7H_{10}O_2)H^+$	5.6	1.5	-	-	0.1
127.11	$(C_8H_{14}O)H^+$	5.5	1.5	1.3	0.7	-
129.06	$(C_6H_8O_3)H^+$	7.6	0.8	2.4	-	0.1
129.09	$(C_7H_{12}O_2)H^+$	-	0.6	1.1	0.3	0.1
129.13	$(C_8H_{16}O)H^+$	-	-	1.2	0.2	0.1
135.08	$(C_9H_{10}O)H^+$	5.6	1.6	1.7	-	-
137.06	$(C_8H_8O_2)H^+$	4.6	0.6	1.4	0.2	0.1
138.06	**$(C_7H_7NO_2)H^+$**	3.8	0.6	-	-	-
139.04	$(C_7H_6O_3)H^+$	4.8	0.6	1.1	0.3	0.1
140.03	**$(C_6H_5NO_3)H^+$**	3.8	0.5	-	0.3	0.1
141.06	$(C_7H_8O_3)H^+$	6.3	0.6	1.7	0.3	0.1
141.13	$(C_9H_{16}O)H^+$	2.5	0.8	-	0.2	-
143.03	$(C_6H_6O_4)H^+$	3.2	0.2	0.6	0.2	0.1
149.02	$(C_8H_4O_3)H^+$	2.3	0.5	1.2	0.3	0.3
152.07	**$(C_8H_9NO_2)H+$**	3.9	0.7	0.3	0.1	-
154.05	**$(C_7H_7NO_3)H^+$**	4.2	-	1.2	0.3	0.1
168.07	**$(C_8H_9NO_3)H^+$**	6.4	0.6	1.8	0.2	-
171.03	$(C_7H_6O_5)H^+$	1.4	0.1	0.1	-	-
173.04	$(C_7H_8O_5)H^+$	3.8	0.1	0.3	-	-
Fraction of the above compounds to the total secondary VOC		**0.89**	**0.96**	**0.97**	**0.97**	**0.96**

Table S4: Supplementary information about SOA composition for the 5 experiments.

Number of experiments	**Exp #1**	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
Type of cycle	**Cold Urban**	**Cold Urban**	**Cold Urban**	**Hot Urban**	**Motorway**
Based on CHARON/PTR-ToF-MS					
Fraction (of ppb) to m/z 200 into SOA	0.98	0.99	0.99	0.99	0.99
Fraction of ON into SOA	0.07	0.06	0.07	0.07	0.07
Based on HR-ToF-AMS					
Fraction of organonitrates into total nitrate	0.15	0.20	0.20	0.12	0.19
Fraction of organoammoniums into total ammonium	NA	0.001	NA	NA	0.13
Ratio cations/anions (inorganic phase)	0.75	1.01	0.99	0.86	1.15
Possible HNO_3 ($\mu g\ m^{-3}$)	23.29	NA	0.09	16.21	NA
Fraction of ammonium and nitrate in total secondary aerosol	0.74	0.79	0.91	0.93	0.79

Table S5: List of the measured accurate *m/z's* and elemental composition $C_xH_yN_zO_w^+$ of the most significant detected ions with concentration higher than 0.14% % of the total SOA concentration produced during cold urban (experiment #1, 2 and 3), hot urban (experiment #4) and motorway (experiment # 5) Artemis cycles. Concentrations are in ppb (before conversion to µg m^{-3} and normalization to the AMS organic mass concentration). These ions explained 79-92% of the measured concentration.

				Concentration (ppb)		
m/z	**Molecular formula**	**Exp #1**	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
31.02	$(CH_2O)H^+$	4.6	0.6	1.5	0.4	-
33.03	$(CH_3OH)H^+$	-	10.3	30.8	20.8	3.8
42.01	$(C_2HO)H^+$	2.6	0.3	-	0.4	0.7
43.02	$C_2H_3O^+$	72	6.7	22.3	8.8	0.5
45.00	$(CO_2)H^+$	1.8	0.9	-	2.5	1.3
45.03	$(C_2H_4O)H^+$	34.4	2.5	8.2	4.2	-
47.01	$(CH_2O_2)H^+$	65.9	6.4	12.5	8.9	0.1
57.03	$(C_3H_4O)H^+$	13.1	0.6	2.4	0.8	0.2
58.03	**$(C_2H_3NO)H^+$**	5.5	0.5	0.8	0.6	-
59.01	$(C_2H_2O_2)H^+$	5.6	-	-	0.9	0.1
59.05	$(C_3H_6O)H^+$	30.7	8.1	8.4	11.8	-
60.04	**$(C_2H_5NO)H^+$**	8.3	1	3.7	2	0.2
61.03	$(C_2H_4O_2)H^+$	57.5	5	22.1	9.8	0.7
65.02	$H_2O(CH_2O_2)H^+$	7.5	0.6	1.8	1.4	-
69.03	$(C_4H_4O)H^+$	2.9	0.2	0.5	0.2	-
71.01	$(C_3H_2O_2)H^+$	6.3	0.3	1	0.5	-
71.05	$(C_4H_6O)H^+$	5.2	0.2	0.8	0.5	0.2
72.04	**$(C_3H_5NO)H^+$**	2	0.2	0.5	0.3	-
73.03	$(C_3H_4O_2)H^+$	38.8	3.3	12.8	5	0.6
74.02	**$(C_2H_3NO_2)H^+$**	8.1	0.6	1.9	1.4	-
74.03	$([13C]C_2H_4O_2)H^+$	2.6	0.2	0.9	-	-
75.01	$(C_2H_2O_3)H^+$	2.2	0.2	0.6	0.3	-
75.04	$(C_3H_6O_2)H^+$	15.7	1.3	5.2	1.7	0.3
76.04	**$(C_2H_5NO_2)H^+$**	2.2	0.2	0.8	0.5	-
77.02	$(C_2H_4O_3)H^+$	4.5	0.3	1.8	0.5	0.1
79.04	$((C_2H_4O_2)H_2O)H^+$	1.7	-	0.2	0.1	-
83.01	$(C_4H_2O_2)H^+$	1.7	0.1	0.3	0.2	-
83.05	$(C_5H_6O)H^+$	5.5	0.2	0.9	0.4	0.1
84.04	**$(C_4H_5NO)H^+$**	1.8	0.1	-	0.2	-
85.03	$(C_4H_4O_2)H^+$	16.1	0.8	2.9	1.2	0.2
85.06	$(C_5H_8O)H^+$	3	0.1	0.6	0.4	0.1
86.03	$([13C]C_3H_4O_2)H^+$	3.6	0.2	0.9	0.5	0.1
87.01	$(C_3H_2O_3)H^+$	3.2	-	-	0.3	0.1
87.04	$(C_4H_6O_2)H^+$	22.9	1.5	6.8	2.5	0.4
88.05	$([13C]C_3H_6O_2)H^+$	-	0.2	0.9	0.4	-
89.02	$(C_3H_4O_3)H^+$	18.2	1	4.4	3.3	0.3
89.06	$(C_4H_8O_2)H^+$	2.3	0.3	1.3	0.8	0.3

90.02	**$(C_2H_3NO_3)H^+$**	6.5	0.7	7.4	2.2	0.8
91.04	$(C_3H_6O_3)H^+$	4.2	0.3	1.1	0.3	-
93.05	$(C_5H_4N_2)H^+$	2	0.2	0.7	0.4	-
95.05	$(C_6H_6O)H_+$	3.4	0.1	0.2	-	0.1
97.03	$(C_5H_4O_2)H^+$	10.8	0.6	1.7	0.9	-
97.06	$(C_6H_8O)H^+$	7.5	0.3	1	0.4	-
98.03	$([13C]C_4H_4O_2)H^+$	4.7	0.3	0.8	0.6	0.1
99.01	$(C_4H_2O_3)H^+$	21.3	1.7	1.6	1.9	0.5
99.04	$(C_5H_6O_2)H^+$	20.3	1.1	4.2	1.6	0.3
100.04	**$(C_4H_5NO_2)H^+$**	5.2	0.3	1	0.8	0.1
101.02	$(C_4H_4O_3)H^+$	18.5	1.3	3.9	2	0.3
101.06	$(C_5H_8O_2)H^+$	6.9	0.4	2.3	0.9	0.2
103.04	$(C_4H_6O_3)H^+$	14	0.7	4	1.3	0.2
104.04	$([13C]C_3H_6O_3)H^+$	2.3	0.2	0.9	0.3	-
105.02	$(C_3H_4O_4)H^+$	7.4	0.4	2.1	0.6	0.2
107.05	$(C_7H_6O)H^+$	6.4	0.1	0.4	0.1	0.1
109.03	$(C_6H_4O_2)H^+$	1.6	0.1	0.2	0.2	-
109.07	$(C_7H_8O)H^+$	5.3	0.2	0.5	-	-
111.04	$(C_6H_6O_2)H^+$	18	0.7	2.6	1	0.1
111.08	$(C_7H_{10}O)H^+$	5.6	0.2	0.6	0.2	-
112.04	**$(C_5H_5NO_2)H^+$**	5.8	0.3	1	0.6	-
113.02	$(C_5H_4O_3)H^+$	24.9	1.9	4.1	1.8	0.4
113.06	$(C_6H_8O_2)H^+$	13.6	0.7	3	1	0.1
114.03	$([13C]C_4H_4O_3)H^+$	3.4	0.2	0.9	0.5	0.1
115.02	$(C_8H_2O)H^+$	4.3	0.1	0.7	0.6	0.3
115.04	$(C_5H_6O_3)H^+$	26.6	2.1	7.7	2.4	0.3
115.08	$(C_6H_{10}O_2)H^+$	2.2	0.2	0.8	0.3	0.1
116.04	**$(C_4H_5NO_3)H^+$**	4.6	0.2	1.2	0.6	0.1
117.02	$(C_4H_4O_4)H^+$	13.5	0.6	1.3	0.7	0.1
117.06	$(C_5H_8O_3)H^+$	6.7	0.5	2.6	0.9	0.2
119.03	$(C_4H_6O_4)H^+$	3.7	0.2	0.6	-	-
123.04	$(C_7H_6O_2)H^+$	4.6	0.2	0.7	0.5	0.5
124.05	$([13C]C_6H_6O_2)H^+$	3.5	0.1	0.5	0.3	0.1
125.02	$(C_6H_4O_3)H^+$	4.1	0.2	0.8	0.4	0.1
125.06	$(C_7H_8O_2)H^+$	11.5	0.5	2.2	0.6	0.1
126.02	$(C_2H_5O_6)H^+$	1.9	0.4	0.6	0.3	-
126.06	$(C_6H_7NO_2)H^+$	3.5	0.2	0.7	0.3	-
127.04	$(C_6H_6O_3)H^+$	18.5	0.9	4.6	1.4	0.2
127.08	$(C_7H_{10}O_2)H^+$	4.7	0.2	0.9	0.3	0.1
128.04	$([13C]C_5H_6O_3)H^+$	2.3	0.2	1.2	0.5	0.1
129.02	$(C_5H_4O_4)H^+$	4.2	0.2	1.1	0.5	0.1
129.06	$(C_6H_8O_3)H^+$	15	0.9	4.3	1.2	0.2
130.04	$(C_9H_5O)H^+$	3.8	0.2	0.7	0.4	-
130.06	$([13C]C_5H_8O_3)H^+$	2.9	0.2	0.8	0.3	-
131.03	$(C_5H_6O_4)H^+$	8.4	0.4	2	0.7	0.1
131.07	$(C_6H_{10}O_3)H^+$	-	-	0.7	0.2	0.1

132.04	$([13C]C_4H_6O_4)H^+$	1.8	-	0.6	0.3	-
133.05	$(C_5H_8O_4)H^+$	4	0.2	1	0.4	-
137.06	$(C_8H_8O_2)H^+$	5.7	0.3	0.8	-	0.1
138.05	**$(C_7H_7NO_2)H^+$**	3.2	0.1	0.3	0.1	0.1
139.04	$(C_7H_6O_3)H^+$	6.8	0.4	1.6	0.6	0.1
139.08	$(C_8H_{10}O_2)H^+$	8.4	0.3	1	0.3	-
140.03	**$(C_6H_5NO_3)H^+$**	4.1	0.2	0.7	0.4	0.1
141.02	$(C_6H_4O_4)H^+$	2.8	-	0.5	0.3	0.1
141.06	$(C_7H_8O_3)H^+$	16.1	0.7	3.9	1.1	0.2
142.06	$([13C]C_6H_8O_3)H^+$	6.2	0.2	1.2	0.5	-
143.03	$(C_6H_6O_4)H^+$	8.1	0.4	2.1	0.8	0.1
143.07	$(C_7H_{10}O_3)H^+$	3.8	0.2	1.1	0.3	0.1
144.04	$([13C]C_5H_6O_4)H^+$	2.9	0.2	0.7	0.3	-
145.05	$(C_6H_8O_4)H^+$	6.5	0.3	1.7	0.5	0.1
149.02	$(C_8H_4O_3)H^+$	6.5	0.5	0.7	1	0.2
151.04	$(C_8H_6O_3)H^+$	2.7	0.1	-	-	0.1
153.06	$(C_8H_8O_3)H^+$	10.4	0.4	2	0.5	0.1
152.07	**$(C_8H_9NO_2)H^+$**	2.1	0.1	0.1	-	-
154.05	**$(C_7H_7NO_3)H^+$**	4.9	0.2	0.8	0.3	0.1
155.03	$(C_7H_6O_4)H^+$	4.6	0.2	0.9	0.3	0.1
155.07	$(C_8H_{10}O_3)H^+$	10.2	0.3	1.8	0.5	0.1
156.03	**$(C_6H_5NO_4)H^+$**	4.2	0.1	0.5	0.3	-
157.05	$(C_7H_8O_4)H^+$	9.6	0.3	2.5	0.6	0.1
159.03	$(C_6H_6O_5)H^+$	4.3	-	0.8	0.3	0.1
161.04	$(C_6H_8O_5)H^+$	2.9	-	0.7	0.2	0.1
163.04	$(C_9H_6O_3)H^+$	3.6	0.2	0.5	0.4	0.2
167.07	$(C_9H_{10}O_3)H^+$	4.6	0.2	0.9	0.2	-
166.05	**$(C_8H_7NO_3)H^+$**	2.6	0.1	0.3	0.1	-
168.07	**$(C_8H_9NO_3)H^+$**	3.7	0.1	0.4	-	0.1
169.05	$(C_8H_8O_4)H^+$	3.6	0.2	1	0.3	-
170.05	**$(C_7H_7NO_4)H^+$**	6.8	0.2	0.6	-	-
171.03	$(C_7H_6O_5)H^+$	2.7	0.1	0.2	0.1	-
171.07	$(C_8H_{10}O_4)H^+$	11.4	0.3	2.2	0.5	0.1
173.04	$(C_7H_8O_5)H^+$	7.9	0.2	1.1	0.3	-
185.08	$(C_9H_{12}O_4)H^+$	4.2	0.1	0.8	-	-
187.06	$(C_8H_{10}O_5)H^+$	7.1	0.1	1.2	0.3	-
Fraction of the above compounds to the total SOA		**0.83**	**0.92**	**0.89**	**0.89**	**0.79**

Table S6: *m/z's* detected in both gas and particle phase, which were used for the gas-to-particle phase partitioning and the corresponding logC^* calculation for each ion for all experiments.

			logC^*				
Number of *m/z*	***m/z***	**Molecular formula**	**Exp #1**	**Exp #2**	**Exp #3**	**Exp #4**	**Exp #5**
1	57.03	$(C_3H_4O)H^+$	4.39	4.64	4.43	3.82	3.90
2	59.01	$(C_2H_2O_2)H^+$	4.00	-	-	-	3.00
3	59.05	$(C_3H_6O)H^+$	5.00	4.53	4.87	3.83	-
4	61.03	$(C_2H_4O_2)H^+$	4.46	4.10	4.52	3.97	4.30
5	71.05	$(C_4H_6O)H^+$	4.60	4.83	4.39	3.85	3.75
6	73.03	$(C_3H_4O_2)H^+$	4.60	4.55	4.37	3.57	3.59
7	75.01	$(C_2H_2O_3)H^+$	3.87	2.87	3.65	3.19	3.05
8	75.04	$(C_3H_6O_2)H^+$	4.28	4.06	4.31	3.70	3.81
9	77.02	$(C_2H_3O_3)H^+$	4.56	4.12	5.00	4.00	3.89
10	83.05	$(C_5H_6O)H^+$	3.90	4.05	3.55	2.99	2.54
11	85.03	$(C_4H_4O_2)H^+$	3.94	3.78	3.59	3.18	3.24
12	85.06	$(C_5H_8O)H^+$	4.56	4.73	4.40	3.83	3.54
13	87.01	$(C_3H_2O_3)H^+$	4.10	3.55	2.69	2.86	2.49
14	87.04	$(C_4H_6O_2)H^+$	4.35	4.38	4.22	3.66	3.57
15	89.06	$(C_4H_8O_2)H^+$	4.49	4.05	4.31	3.77	3.56
16	91.04	$(C_3H_6O_3)H^+$	3.54	-	4.16	3.23	3.74
17	95.05	$(C_6H_6O)H^+$	4.04	4.54	-	-	2.77
18	97.03	$C_5H_4O_2H^+$	4.11	3.73	3.97	3.18	3.97
19	97.06	$(C_6H_8O)H^+$	3.83	3.92	3.61	2.95	3.41
20	99.01	$(C_4H_2O_3)H^+$	4.00	3.67	4.54	3.27	3.41
21	101.02	$(C_4H_4O_3)H^+$	3.80	3.36	3.79	3.25	3.45
22	101.06	$(C_5H_8O_2)H^+$	4.31	4.30	4.08	3.59	3.39
23	103.04	$(C_4H_6O_3)H^+$	3.85	3.33	3.43	2.94	3.04
24	103.08	$(C_5H_{10}O_2)H^+$	-	-	-	3.64	3.30
25	105.02	$(C_3H_4O_4)H^+$	3.60	3.42	3.05	2.59	2.67
26	107.05	$(C_7H_6O)H^+$	4.28	4.50	4.61	-	2.97
27	109.07	$(C_7H_8O)H^+$	3.98	4.55	3.65	3.33	3.49
28	111.04	$(C_6H_6O_2)H^+$	4.02	3.80	3.79	3.02	2.99
29	113.02	$(C_5H_4O_3)H^+$	4.22	3.87	4.24	3.39	3.46
30	113.06	$(C_6H_8O_2)H^+$	4.54	4.69	4.01	3.48	3.48
31	115.04	$(C_5H_6O_3)H^+$	3.85	3.40	3.59	3.06	3.31
32	115.08	$(C_6H_{10}O_2)H^+$	4.48	4.46	4.34	3.86	3.46
33	117.02	$(C_4H_4O_4)H^+$	3.44	3.05	3.47	2.90	3.00
34	117.06	$(C_5H_8O_3)H^+$	3.62	2.91	3.59	2.94	2.67
35	119.03	$(C_4H_6O_4)H^+$	3.72	3.00	3.54	3.13	3.36
36	121.07	$(C_8H_8O)H^+$	4.27	5.00	4.90	-	-
37	123.04	$(C_7H_6O_2)H^+$	4.04	3.95	4.24	3.25	2.93
38	123.08	$(C_8H_{10}O)H^+$	4.35	5.05	-	-	2.99
39	125.02	$(C_6H_4O_3)H^+$	3.95	3.70	4.04	3.35	3.64
40	125.06	$(C_7H_8O_2)H^+$	3.88	3.62	3.58	3.02	3.06
41	127.04	$(C_6H_6O_3)H^+$	3.96	3.74	3.75	3.11	3.31
42	127.08	$(C_7H_{10}O_2)H^+$	4.29	4.46	3.85	3.36	3.29
43	129.02	$(C_5H_4O_4)H^+$	4.04	3.44	3.56	3.11	2.99
44	129.06	$(C_6H_8O_3)H^+$	3.92	3.58	3.66	2.55	2.93
45	131.03	$(C_5H_6O_4)H^+$	3.60	3.35	3.29	2.89	2.79
46	133.05	$(C_5H_8O_4)H^+$	3.67	3.55	3.19	2.67	2.43

47	135.05	$(C_8H_6O_2)H^+$	3.89	3.22	2.75	-	1.73
48	135.08	$(C_9H_{10}O)H^+$	4.03	4.27	-	-	3.17
49	137.06	$(C_8H_8O_2)H^+$	4.12	3.97	4.15	3.70	3.51
50	138.06	**$(C_7H_7NO_2)H^+$**	4.66	-	-	-	-
51	139.04	$(C_7H_6O_3)H^+$	4.06	3.85	3.76	3.29	3.15
52	139.08	$(C_8H_{10}O_2)H^+$	3.90	3.93	3.56	3.02	3.13
53	140.03	**$(C_6H_5NO_3)H^+$**	4.18	3.93	3.92	3.46	3.23
54	141.06	$(C_7H_8O_3)H^+$	3.81	3.57	3.55	3.01	3.11
55	143.03	$(C_6H_6O_4)H^+$	3.81	3.41	3.35	2.93	2.77
56	145.05	$(C_6H_8O_4)H^+$	3.74	3.39	3.26	2.74	2.75
57	147.03	$(C_5H_6O_5)H^+$	3.90	-	3.29	-	2.37
58	149.04	$(C_5H_8O_5)H^+$	-	-	3.75	-	3.79
59	151.08	$(C_9H_{10}O_2)H^+$	3.97	3.88	3.93	-	3.17
60	152.07	**$(C_8H_9NO_2)H^+$**	4.49	-	-	-	-
61	153.06	$(C_8H_8O_3)H^+$	3.85	3.65	3.38	2.43	2.40
62	154.05	**$(C_7H_7NO_3)H^+$**	4.15	3.96	4.09	3.63	3.30
63	155.03	$(C_7H_6O_4)H^+$	4.03	3.65	3.54	3.01	2.84
64	155.07	$(C_8H_{10}O_3)H^+$	3.87	3.82	3.56	3.17	2.89
65	157.05	$(C_7H_8O_4)H^+$	3.73	3.35	3.29	2.86	2.90
66	168.07	**$(C_8H_9NO_3)H^+$**	4.45	4.42	4.56	-	3.45
67	170.05	**$(C_7H_7NO_4)H^+$**	3.61	3.20	3.32	2.85	-
68	173.04	$(C_7H_8O_5)H^+$	3.90	3.51	3.32	2.83	2.61
69	181.05	$(C_9H_8O_4)H^+$	3.97	3.56	3.28	-	2.49

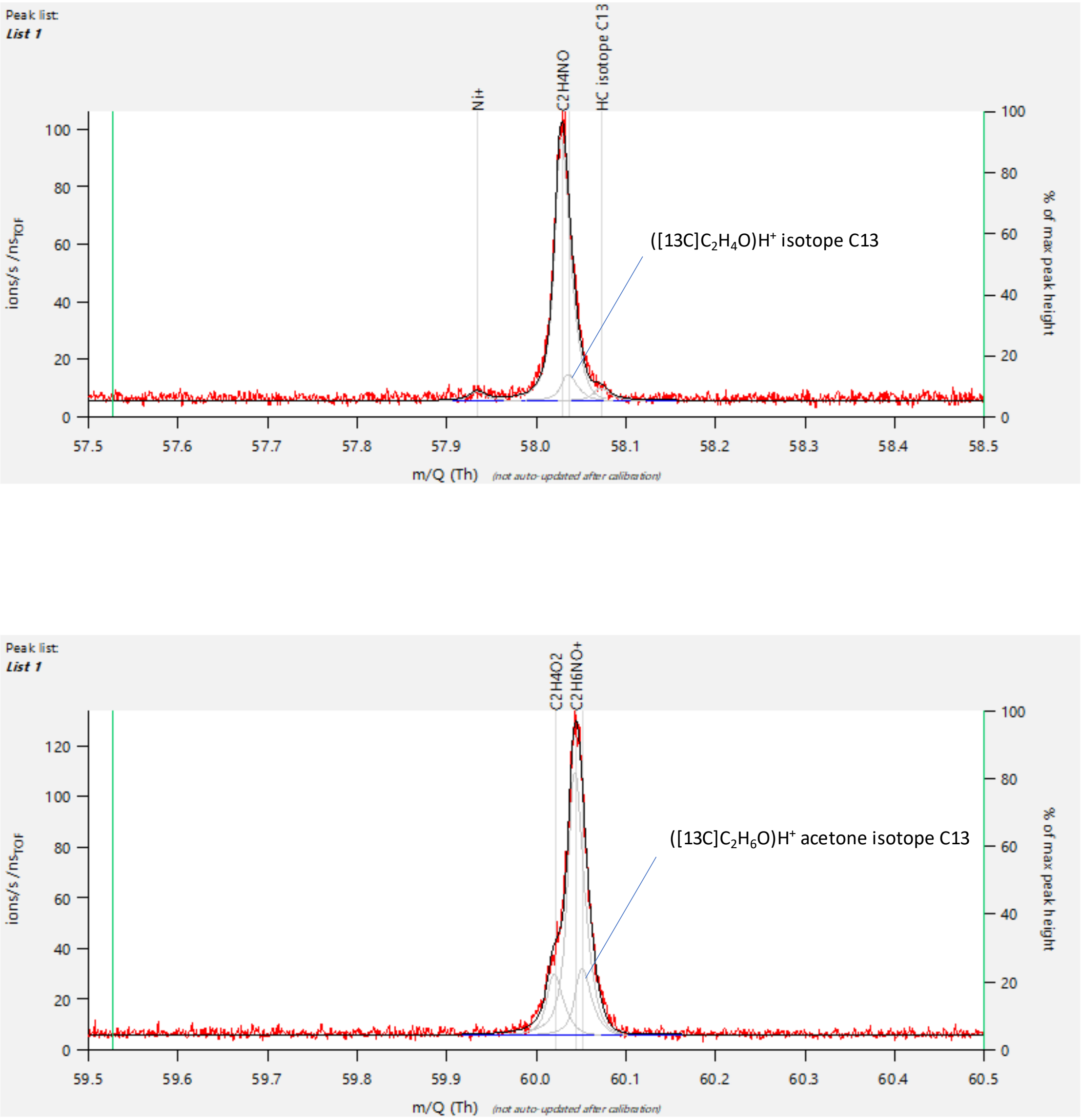

Figure S1: Examples of CHARON mass spectra containing ON at *m/z* 58 (top) and *m/z* 60 (bottom). The contribution of the isotopes was present but clearly distinguished from the ON.

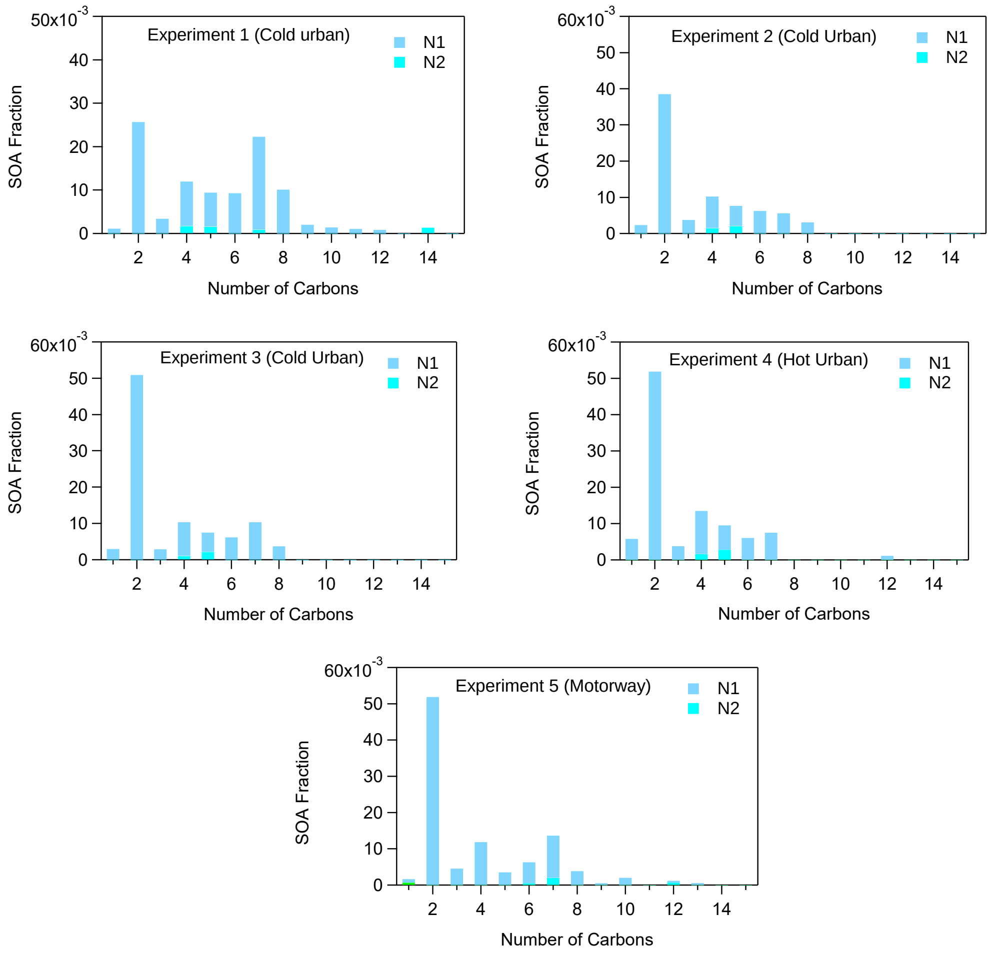

Figure S2: N to C distributions for the SOA formed during each one of the five experiments.

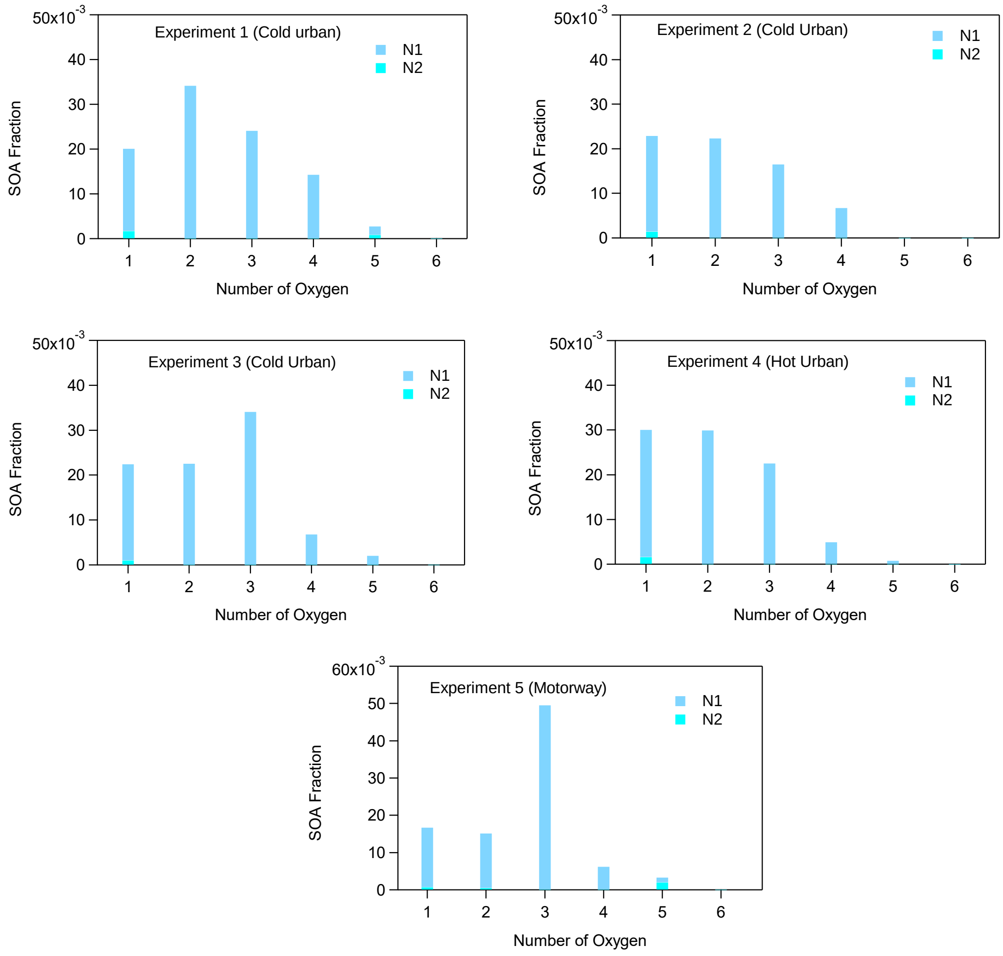

Figure S3: N to O distributions for the SOA formed during each one of the five experiments.

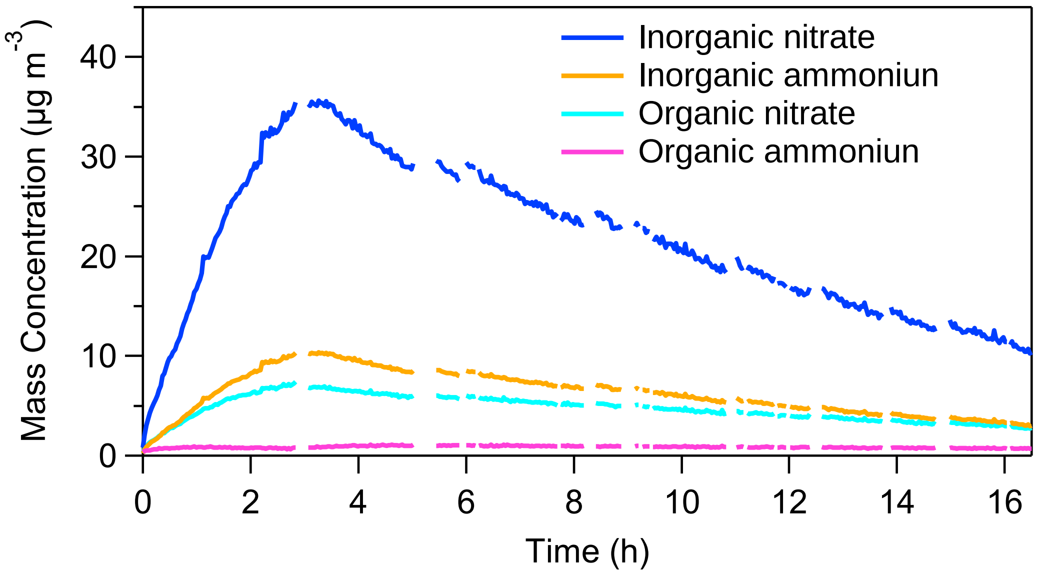

Figure S4: Time-series of inorganic nitrate, inorganic ammonium, organic nitrate and organic ammonium mass concentrations for the experiment #5 (photo-oxidation of motorway emissions). Time zero corresponds to the moment where the photo-oxidation begins.

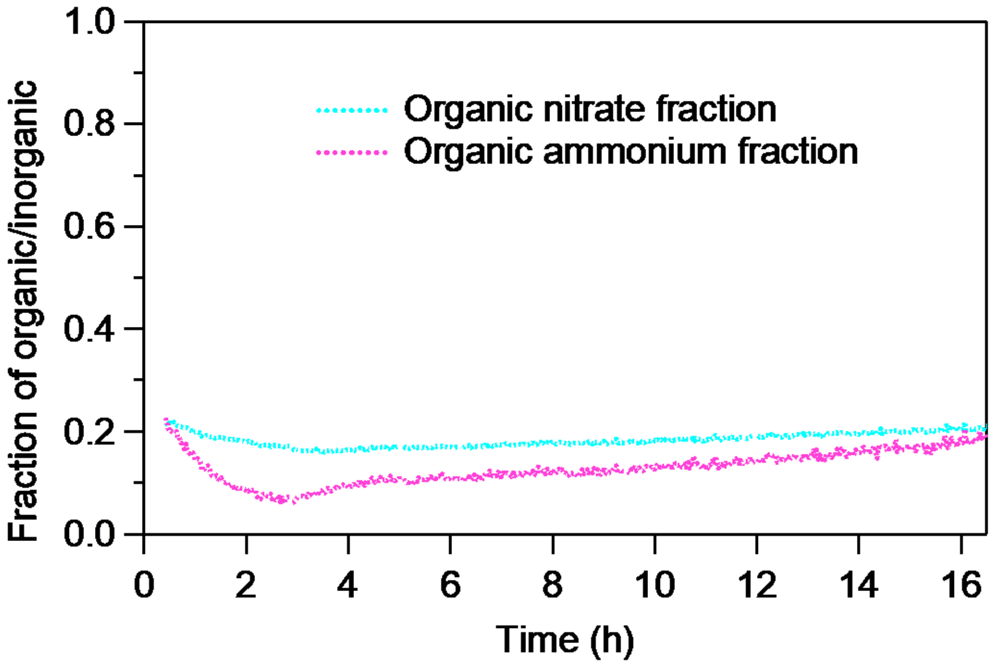

Figure S5: Mass fraction of organic nitrate and organic ammonium over the total nitrate and ammonium mass concentrations respectively for the experiment #5 (photo-oxidation of motorway emissions).

References

Bosque, R.; and Sales, J.: Polarizabilities of solvents from the chemical composition, J. Chem. Inf. Comput. Sci., 42 (5), 1154−1163, 2002.

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

Gioumousis, G.; Stevenson, D. P.: Reactions of gaseous molecule ions with gaseous molecules. v. theory, J. Chem. Phys., 29, 294−299, 1958.

Langevin, P. J. : Recombination et mobilités des ions dans les gaz, Ann. Chim. Phys., 28, 433−530, 1903.

Su, T.; Chesnavich, W. J.: Parametrization of the ion–polar molecule collision rate constant by trajectory calculations, J. Chem. Phys., 76, 5183−5185, 1982.