

Supplemental Information

Comparison of Methods of Functional Group Analysis Using Results from Laboratory and Field Aerosol Measurements

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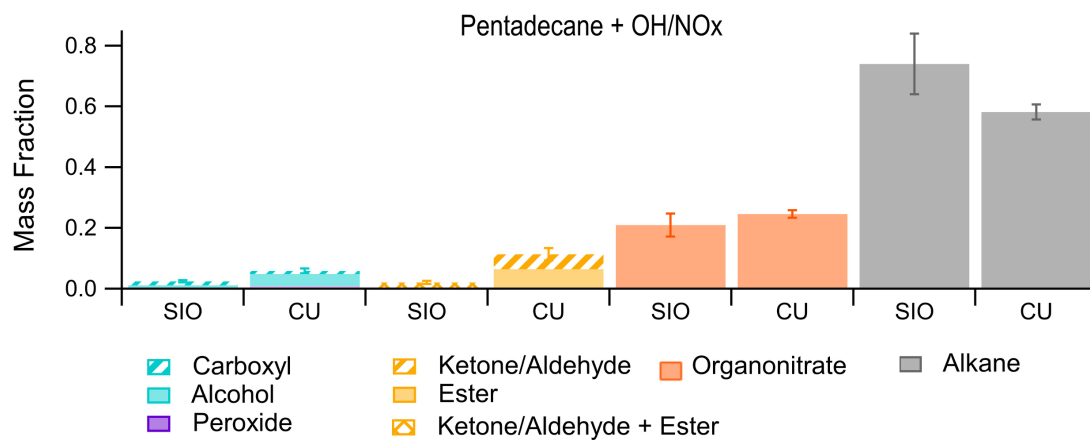


Figure S1. Functional group composition of SOA formed in the environmental chamber reaction of pentadecane with OH radicals in the presence of NO_x. This corresponds to experiment 5 in Table 1.

Table S1. Functional group composition of the SOA formed from the reaction of selected monoterpenes with NO₃ radicals and analyzed using the Deriv-Spec methods.

	Limonene	α -Pinene	β -Pinene	β -Pinene ^a
Functional Group	Functional Group / C ₁₀ Molecule			
Carboxyl [O=COH]	0.00	0.00	0.06	0.04
Ketone/Aldehyde [C=O]	0.17	0.18	0.43	0.28
Ester [O=COR]	0.17	0.04	0.01	0.12
Hydroxyl [HCOH]	0.02	0.05	0.00	0.08
Peroxide [HCOOH]	0.03	0.01	0.02	0.06
Nitrate [HCONO ₂]	1.05	0.71	1.12	0.76
Methylene [CH ₂]	8.56	9.00	8.37	8.65
O/C	0.37	0.25	0.40	0.31
H/C	1.83	1.88	1.80	1.84
N/C	0.10	0.07	0.11	0.08
MW	213	188	217	199
C* ($\mu\text{g m}^{-3}$)	5×10^4	1×10^5	1×10^4	5×10^4
Density (g/mL)	1.19	1.07	1.21	1.12

^a SOA formed in presence of (NH₄)₂SO₄/H₂SO₄ seed.

Table S2. Functional group composition of the SOA formed from the reaction of VOCs with OH/NO_x, OH, or with O₃ and analyzed by the Deriv-Spec methods.

	Pentadecane	Isoprene	α -Pinene	α -Pinene	α -Pinene ^a
	OH/NO _x		OH		O ₃
Functional Group	Functional Group / C ₁₀ Molecule				
Carboxyl [O=COH]	0.07	0.28	0.08	0.68	1.62
Ketone/Aldehyde [C=O]	0.52	0.32	0.69	1.03	1.66
Ester [O=COR]	0.45	0.61	0.65	0.26	0.71
Hydroxyl [HCOH]	0.40	0.28	0.23	0.28	0.14
Peroxide [HCOOH]	0.06	0.04	0.08	1.03	0.13
Nitrate [HCONO ₂]	0.99	0.33	0.55	0.00	0.00
Methylene [CH ₂]	12.52	3.14	7.07	6.73	5.74
O/C	0.34	0.69	0.42	0.52	0.67
H/C	1.80	1.51	1.54	1.67	1.36
N/C	0.07	0.07	0.06	0.00	0.00
MW	301	127	203	221	241
C* ($\mu\text{g m}^{-3}$)	10	1×10^6	1×10^4	3×10^3	0.1
Density (g/mL)	1.14	1.45	1.27	1.26	1.45

^a SOA formed in the absence of seed.

Micro-Method Hydroxyl Group Analysis

Hydroxyl analysis used the following solutions: 3:2 v/v toluene/methanol; 8 mM trimethylsilyldiazomethane (TMSDM) made from 0.4 M TMSDM in diethyl ether and 3:2 v/v toluene/methanol solution; 0.2 M dinitrobenzoyl chloride (3,5-DNBC) in pyridine; 0.6 M NaHCO_3 in water; 0.24 N HCl and 0.9 M NaCl in water; 23:2 v/v hexane/dichloromethane (DCM). The procedure was as follows: a sample or standard solution containing at least 0.07 nmol of hydroxyl groups dissolved in 5 μL of toluene/methanol solution is added to a 0.5 mL conical glass reaction vial with 10 μL of TMSDM solution. The solution is kept at room temperature for 1 h to convert any carboxyl groups to methyl esters, and is then dried in a stream of UHP N_2 . The sample is then reconstituted into 5 μL pyridine and 7.5 μL of 3,5-DNBC solution and left at room temperature for 15 min to allow time for derivatization. To hydrolyze any excess 3,5-DNBC, 25 μL of water is added to the sample and the solution is kept at room temperature for 10 min. The sample is then dried in a stream of UHP N_2 . Once dried, each sample is reconstituted in 250 μL of hexane/DCM solution. The sample is then washed with 100 μL of NaHCO_3 solution followed by 250 μL of HCl/NaCl solution, after each washing the aqueous layer is discarded. The remaining organic layer is then dried in a stream of UHP N_2 , reconstituted into 25 μL of acetonitrile, and the absorbance is measured at 231 nm.