

Supplement of Atmos. Chem. Phys., 18, 5467–5481, 2018
<https://doi.org/10.5194/acp-18-5467-2018-supplement>
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Supplement of

Characterization of organic nitrate constituents of secondary organic aerosol (SOA) from nitrate-radical-initiated oxidation of limonene using high-resolution chemical ionization mass spectrometry

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Most Prevalent Species

Although 196 individual ions were identified during desorptions of limonene SOA during experiments, a majority of the organic signal can be explained by approximately half of the ions. For example, the 40th percentile of ions based on average signal during desorptions (117 ions) accounted for 93.5% of the signal in the CIMS. Table S1 shows the corresponding membership of each ion in the 40th, 75th and 90th percentile of ions. One caveat to this approach is that it assumes an equal sensitivity across all species, which may introduce some uncertainty into the calculation of each ion's contribution to the organic signal detected in the condensed phase. The ions with same molecular formula as species in the MCM have been identified. For several of these there are multiple entries in MCM that have same molecular mass.

Table S1: The full set of ions detected during desorptions across all experiments and the corresponding composition of the 40th, 75th, and 90th percentile subsets. Note that molecules were detected as iodide clusters (MI)

Molecule	Quantile			Average % Contribution	MCM compound
	40th	75th	90th		
C10H15NO6	x	x	x	11.6	C923PAN
C10H18N2O8	x	x	x	7.8	
C10H15NO7	x	x	x	6.8	
C10H16N2O8	x	x	x	4.8	
C8H11NO7	x	x	x	3	C727PAN C731PAN
C20H29NO16	x	x	x	2.3	
C10H17NO6	x	x	x	1.9	NLIMALOH LIMALNO3
C20H29NO15	x	x	x	1.9	
C10H15NO8	x	x	x	1.9	
C20H29NO17	x	x	x	1.7	
C19H28N2O13	x	x	x	1.6	
C19H27NO15	x	x	x	1.5	
C8H12O4	x	x	x	1.5	C818CO C825CO C729CO3H C731CO2H
C10H17NO7	x	x	x	1.4	NLIMALOOH
C11H17NO11	x	x	x	1.3	

C9H14O4	x	x	x	1.1	C926OH LMKOOA LMKOOB LMKBOO C816CO3H LIMONIC LMLKAOH KLIMONONIC LIMALOOA LMLKBOH C822CO3H
C7H11NO5	x	x	x	1.1	C731NO3
C9H13NO7	x	x	x	1.1	C817PAN C823PAN
C8H11NO6	x	x	x	1	C729PAN
C10H13NO7	x	x	x	1	
C19H28N2O14	x	x		1	
C10H17NO8	x	x		1	
C9H15NO7	x	x		0.9	
C10H16N2O9	x	x		0.8	
C20H24N2O9	x	x		0.8	
C20H27NO15	x	x		0.8	
C20H29NO14	x	x		0.8	
C19H28N2O12	x	x		0.8	
C20H27NO16	x	x		0.8	
C10H15NO9	x	x		0.7	
C18H26N2O12	x	x		0.7	
C9H13NO8	x	x		0.7	
C20H27NO17	x	x		0.7	
C10H16O4	x	x		0.7	LIMALBOOH C923CO3H LIMALAOOH
C20H24N2O8	x	x		0.6	
C20H22N2O8	x	x		0.6	
C17H25NO15	x	x		0.6	
C17H23NO14	x	x		0.6	
C19H28N2O11	x	x		0.6	
C6H13NO10	x	x		0.6	
C9H13NO9	x	x		0.5	
C10H15NO5	x	x		0.5	
C9H15NO5	x	x		0.5	LMKANO3 LMKBNO3
C8H13NO7	x	x		0.5	NC826OOH
C7H10O4	x	x		0.5	C735OH C732CO C626CO2H C733CO C735OOA CO25C6CO2H

C19H28N2O15	x	x		0.5	
C16H23N3O14	x	x		0.5	
C9H13NO6	x	x		0.5	C816PAN C822PAN
C7H11NO6	x	x		0.4	C624PAN C732NO3 C622PAN
C20H24N2O10	x	x		0.4	
C18H28N2O12	x	x		0.4	
C19H26N2O13	x	x		0.4	
C10H18N2O9	x			0.4	
C7H9NO7	x			0.4	C626PAN C627PAN
C20H22N2O9	x			0.4	
C19H27NO17	x			0.4	
C10H14O9	x			0.4	
C11H15NO11	x			0.4	
C8H10O4	x			0.4	
C11H14O10	x			0.4	
C20H28N2O17	x			0.3	
C8H10O9	x			0.3	
C20H22N2O10	x			0.3	
C10H17NO5	x			0.3	NLIMOOH
C8H11NO8	x			0.3	C732PAN
C10H17NO9	x			0.3	
C20H21NO7	x			0.3	
C16H24N2O10	x			0.3	
C18H26N2O14	x			0.3	
C20H21NO6	x			0.3	
C18H26N2O15	x			0.3	
C20H27NO14	x			0.3	
C10H14O6	x			0.3	
C11H14O9	x			0.3	
C10H14N2O9	x			0.3	
C8H13NO8	x			0.3	
C18H26N2O11	x			0.3	
C10H13NO6	x			0.3	
C10H14O5	x			0.3	
C19H26N2O11	x			0.3	
C8H12O5	x			0.3	C731CO3H C727CO3H KLIMONIC

C20H22N2O7	x			0.3	
C10H16N2O7	x			0.3	
C19H22N2O8	x			0.3	
C20H23NO7	x			0.3	
C10H12O11	x			0.3	
C19H28N2O10	x			0.3	
C8H12O7	x			0.2	
C9H15NO8	x			0.2	
C22H26N2O9	x			0.2	
C10H14N2O10	x			0.2	
C20H22N2O11	x			0.2	
C7H13NO5	x			0.2	
C10H16O8	x			0.2	
C7H9NO6	x			0.2	
C19H27NO12	x			0.2	
C9H15NO6	x			0.2	NLMKAOOH
C8H12O8	x			0.2	
C8H8O10	x			0.2	
C22H26N2O8	x			0.2	
C10H16N2O11	x			0.2	
C18H24N2O16	x			0.2	
C10H16N2O10	x			0.2	
C10H12O9	x			0.2	
C10H14O11	x			0.2	
C7H11NO7	x			0.2	
C20H23NO6	x			0.2	
C8H12N2O9	x			0.2	
C16H21N3O14	x			0.2	
C9H14O5	x			0.2	C926OOH LMLKBOOH C823CO3H C817CO3H LMLKAOOH
C19H26O14	x			0.2	
C20H23NO5	x			0.2	
C19H26N2O12	x			0.2	
C20H32N2O11	x			0.2	
C19H27NO11	x			0.2	
C18H24N2O17	x			0.2	
C8H12O9	x			0.1	

C10H14O8				0.1	
C8H11NO10				0.1	
C20H23NO8				0.1	
C7H9NO5				0.1	
C6H13NO9				0.1	
C10H16O5				0.1	
C10H14O4				0.1	
C6H13NO11				0.1	
C20H26O18				0.1	
C18H24N2O18				0.1	
C20H32N2O10				0.1	
C18H28N2O11				0.1	
C10H14O7				0.1	
C10H13NO9				0.1	
C20H21NO10				0.1	
C20H21NO5				0.1	
C10H16O9				0.1	
C20H21NO8				0.1	
C20H20N2O8				0.1	
C20H28N2O16				0.1	
C16H23O9				0.1	
C9H13NO5				0.1	
C22H26N2O7				0.1	
C19H26N2O10				0.1	
C11H14O8				0.1	
C18H24N2O19				0.1	
C20H29NO11				0.1	
C9H12O4				0.1	LMLKBCO LMLKACO
C19H22N2O9				0.1	
C10H14O12				< 0.1	
C10H15NO12				< 0.1	
C10H16N2O13				< 0.1	
C10H16N2O15				< 0.1	
C10H16N2O17				< 0.1	
C10H16N2O19				< 0.1	
C10H16O10				< 0.1	
C10H16O11				< 0.1	
C10H16O12				< 0.1	

C10H16O3				< 0.1	LIMALBOH LIMONONIC LIMOOB LIMOOA LIMALAOH LIMBOO
C10H16O6				< 0.1	
C10H18N2O10				< 0.1	
C10H18N2O7				< 0.1	
C10H18O4				< 0.1	LIMALOH
C14H13NO10				< 0.1	
C15H21NO10				< 0.1	
C15H21NO8				< 0.1	
C16H22O7				< 0.1	
C16H23NO7				< 0.1	
C16H24N2O9				< 0.1	
C18H26N2O10				< 0.1	
C18H26O5				< 0.1	
C18H30O5				< 0.1	
C18H31O7				< 0.1	
C19H22N2O10				< 0.1	
C19H22N2O7				< 0.1	
C19H25NO14				< 0.1	
C19H28N2O9				< 0.1	
C20H20N2O10				< 0.1	
C20H23NO4				< 0.1	
C20H29NO12				< 0.1	
C20H29NO13				< 0.1	
C20H29NO18				< 0.1	
C20H30N2O11				< 0.1	
C20H30N2O9				< 0.1	
C20H32N2O6				< 0.1	
C20H32N2O7				< 0.1	
C20H32N2O8				< 0.1	
C20H32N2O9				< 0.1	
C8H10O10				< 0.1	
C8H10O6				< 0.1	
C8H11NO5				< 0.1	
C8H11NO9				< 0.1	
C8H12O10				< 0.1	
C8H12O6				< 0.1	C820OOH C732CO3H

	C8H8O9				< 0.1	
	C8H9NO12				< 0.1	
	C9H11NO11				< 0.1	
	C9H16O6				< 0.1	C92500H
	C9H15NO9				< 0.1	
	N-containing	-	-	-	87.7	
Total Ions	196	117	52	20	-	
% of ions	100%	59.70%	26.50%	10.20%	-	
Average contribution to Organic Signal	100%	93.50%	75.50%	56.20%	-	

Figure S1 illustrate the particle to gas ratios of ion counts for the low mass range (monomers), Fig S1a and high mass range (dimers) Fig S1b. Most ions had ratios higher than one and were mostly found in the condensed phase.

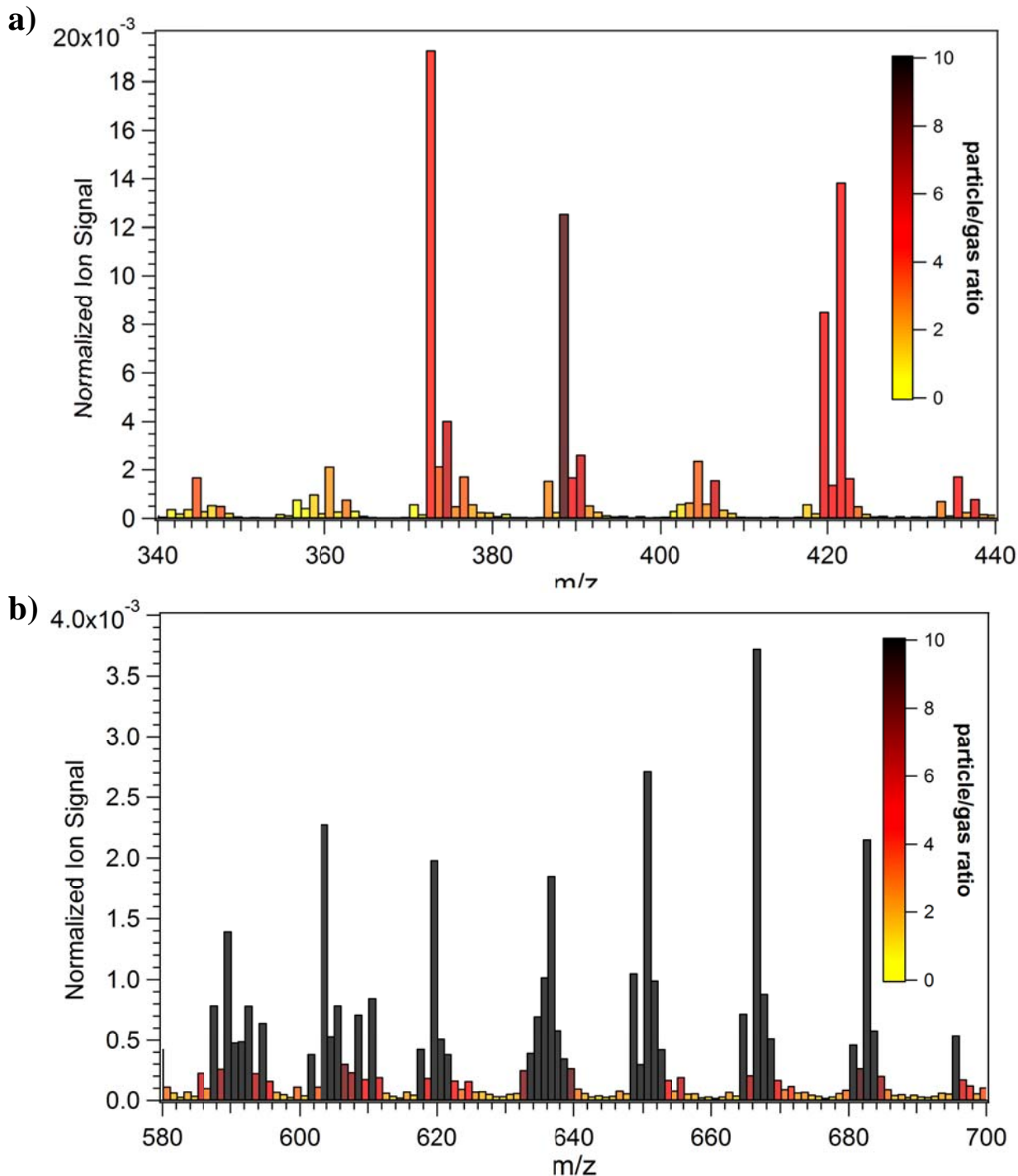


Figure S1. Particle to gas ratio of ions in a) the low MW range (monomers) and b) high MW range (dimers). For particle/gas ratios larger than 10 the color of the bars are black.

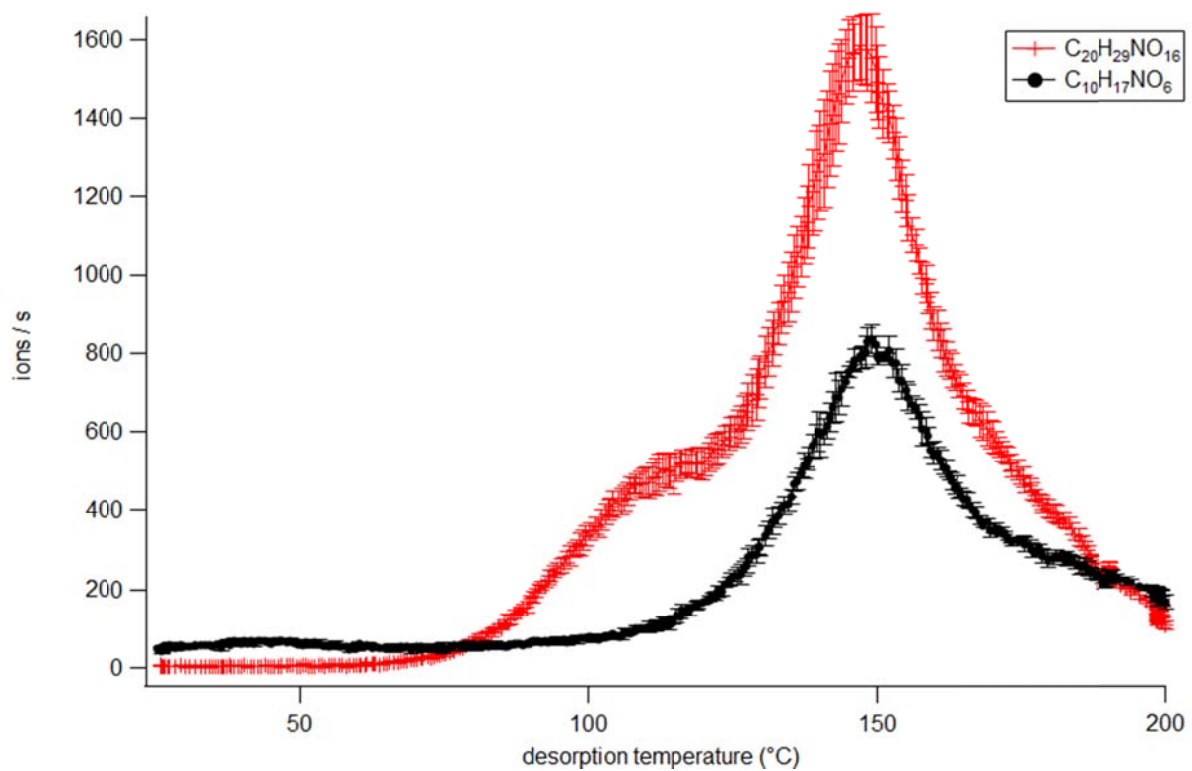


Figure S2. Two desorption profiles illustrating the average of four sequential desorptions with standard deviation provided as error bars.