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Supplement of

Using collision-induced dissociation to constrain sensitivity of ammonia chemical ionization mass spectrometry (NH_4^+ CIMS) to oxygenated volatile organic compounds

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1 Detection of particle phase organics using gas phase denuder and thermal desorption unit

In order to find the optimal temperature for the thermal desorption unit (TDU), we conduct a series of experiments with ammonia sulfate seeds coated with alpha-pinene ozonolysis products. We monitor the particle concentration after the thermal desorption unit using Scanning Mobility Particle Sizer Spectrometer (SMPS, TSI Incorporated) while increasing the temperature of TDU. The results are presented on Fig R1 below. The majority of particles is evaporated at temperatures above 140°C.

We study thermal decomposition of OVOCs extracted from alpha-pinene SOA by measuring their peak intensities using NH_4^+ -CIMS. Signals of many species increase at moderate temperatures ($T < 160^\circ\text{C}$) and level out or decrease at higher temperatures ($T > 180^\circ\text{C}$), as shown in Fig R2. Therefore, we choose the TDU temperature to be 180°C , as at this temperature all particles are evaporated while thermal decomposition of labile species is relatively small.

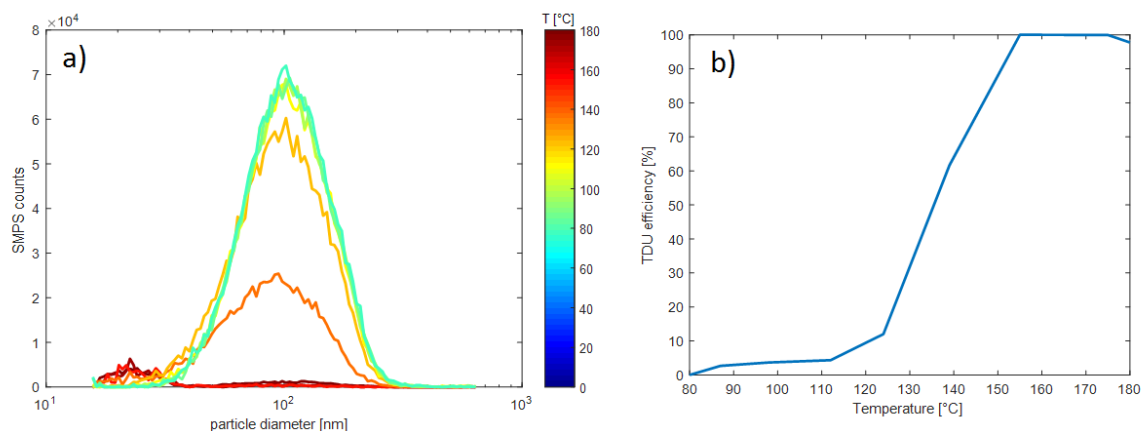


Figure S1: (a) Particle distribution measured by SMPS as a function of temperature of the thermal desorption unit of the NH_4^+ -CIMS; (b) Percentage of particles evaporated in the thermal desorption unit as a function of temperature of the unit.

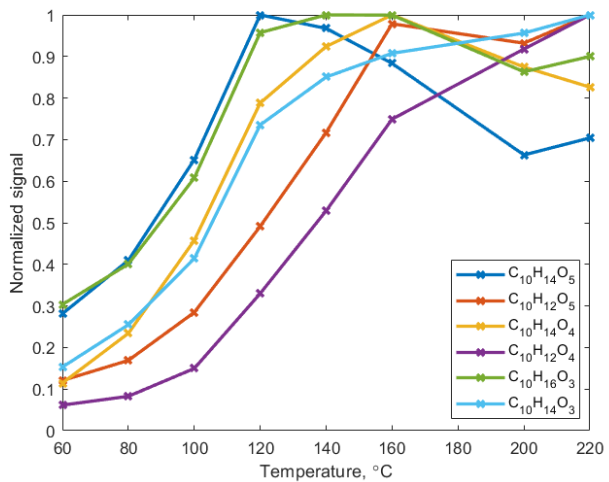


Figure S2: Thermograms of selected alpha-pinene ozonolysis SOA.

2 Additional Figures

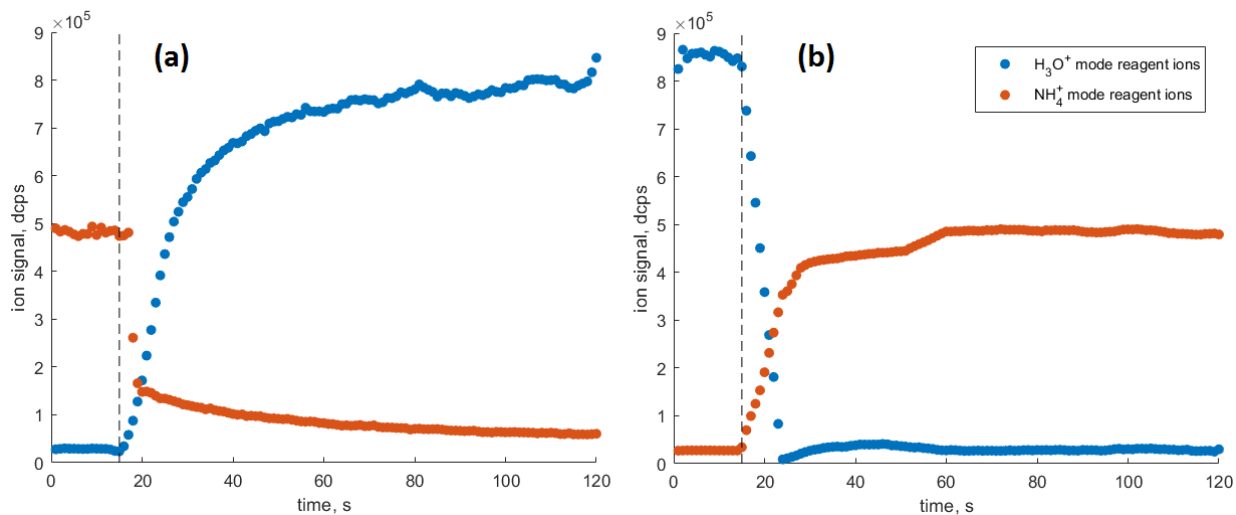


Figure S3: Signals of reagent ions during switching between the two modes. H_3O^+ mode reagent ions comprise $\text{H}_3\text{O}^+(\text{H}_2\text{O})_n$, $n=0,1$; NH_4^+ mode reagent ions comprise $\text{NH}_4^+(\text{H}_2\text{O})_n$, $n=0,1,2$. (a) Switching from the NH_4^+ mode to the H_3O^+ mode. Switching effectively occurs within two minutes. (b) Switching from the H_3O^+ mode to the NH_4^+ mode. Switching effectively occurs within one minute.

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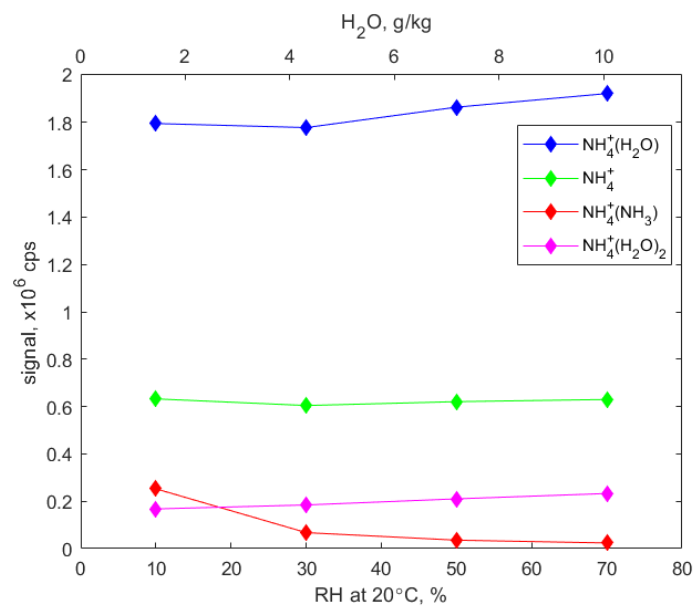


Figure S4: Reagent ion signals as a function of water vapour mixing ratios of the sampled air.

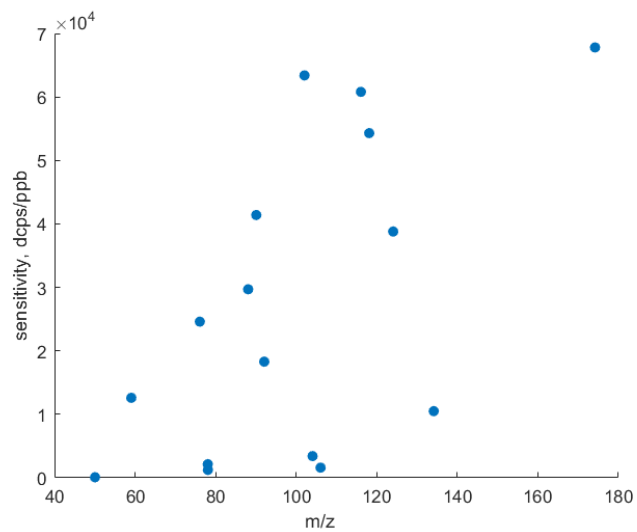


Figure S5: The relationship between the measured sensitivity for calibrated compounds and their molecular weight.

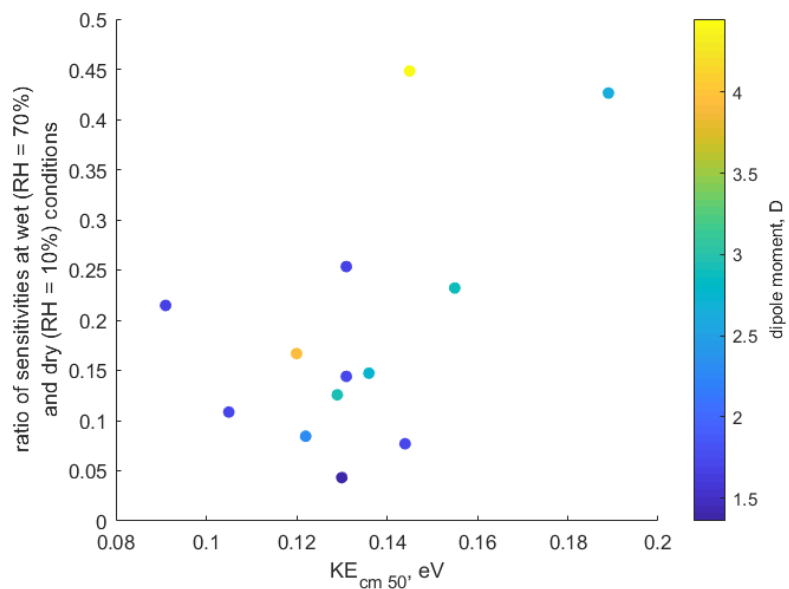


Figure S6: The relationship between the NH_4^+ -CIMS sensitivity dependence on RH and $\text{KE}_{\text{cm } 50}$. Data points are color-coded using the permanent dipole moment of the species.

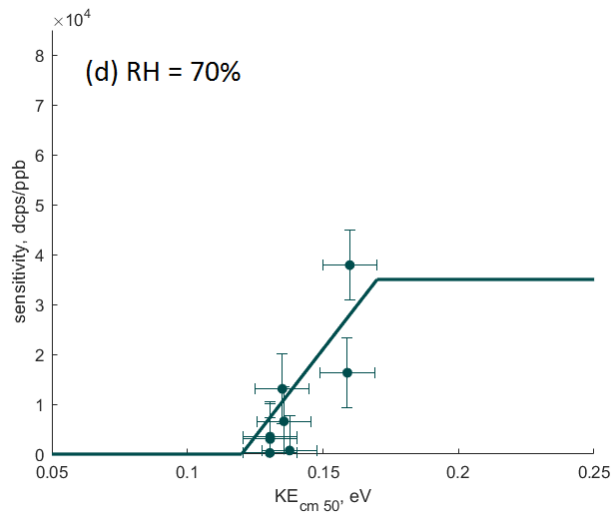
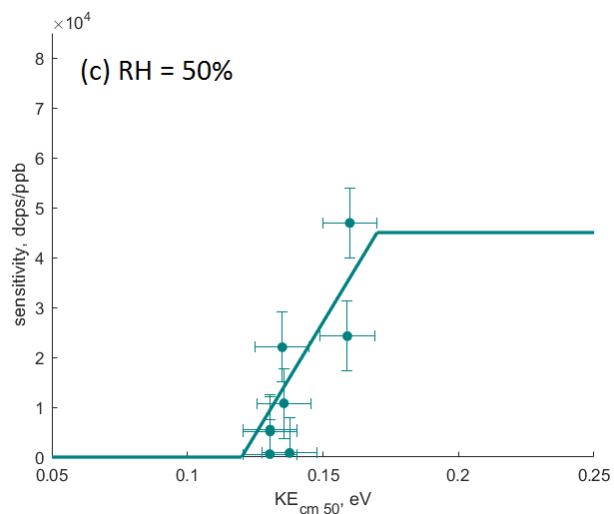
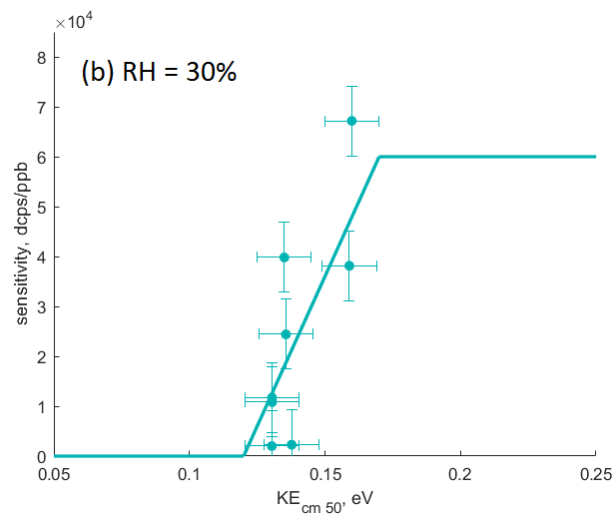
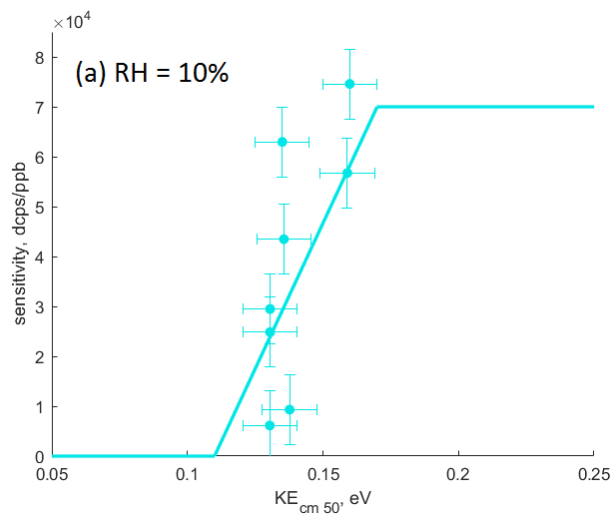


Figure S7: The relationship between calculated kinetic energy of the ammonium-organic clusters $KE_{cm 50}$ and measured sensitivity to calibrated compounds obtained at different RH of the sampled air.

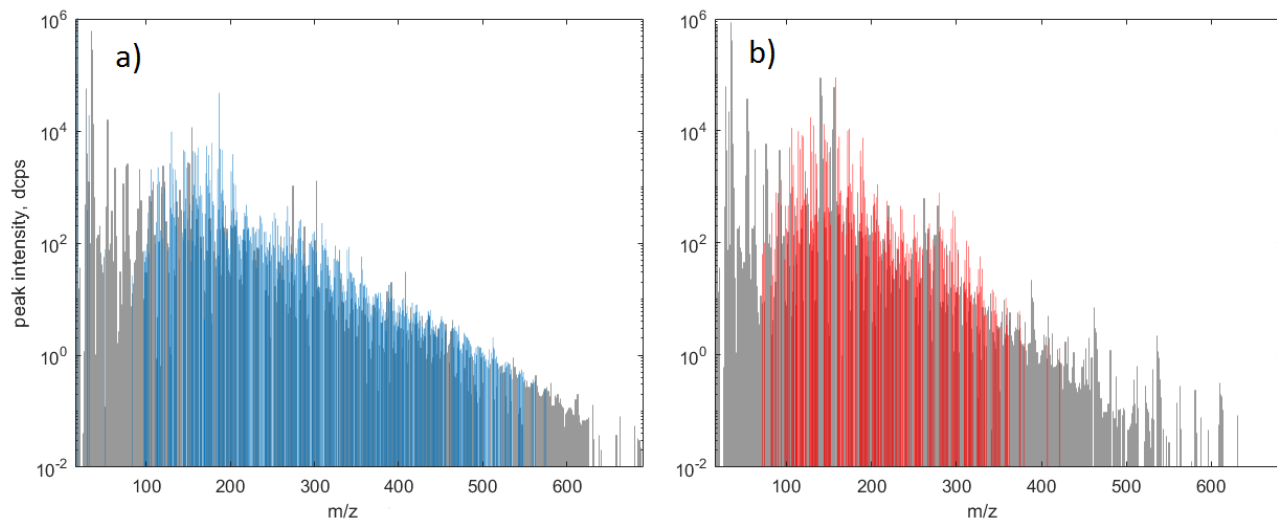


Figure S8: High-resolution mass-spectra obtained during photooxidation of 3-methylcatechol in (a) gas and (b) particle phases. Highlighted peaks are the ones that are enhanced during the experiment.

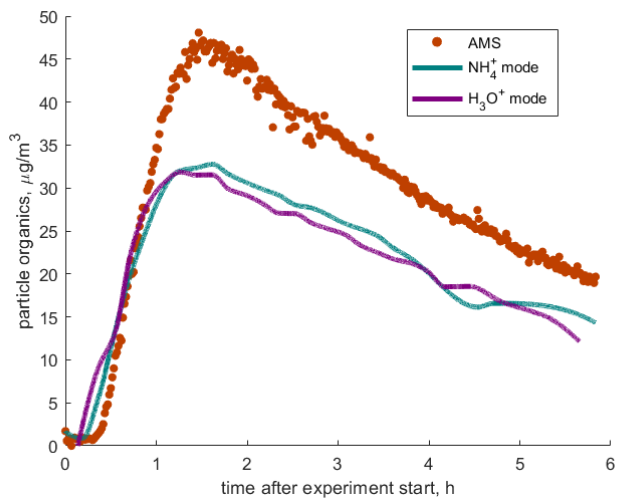


Figure S9: SOA produced during photooxidation of 3-methylcatechol in a laboratory experiment. The total organic mass measured by AMS and the two modes of the CIMS instrument is presented.