Supplementary of

Ammonium CI-Orbitrap: a tool for characterizing the reactivity of oxygenated organic molecules

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Table S1 Main experimental conditions of selected runs analyzed by NH_4^+-Orbitrap.

Run	α-pinene (ppbv)	O_3 (ppbv)	NO_x (ppbv)	CO (ppbv)	SO_2 (ppbv)	RH (%)	T (℃)
2211	2	110	0	130	0	10→80	-10
2213	0.41	110	1.75	1000	0	20	-10

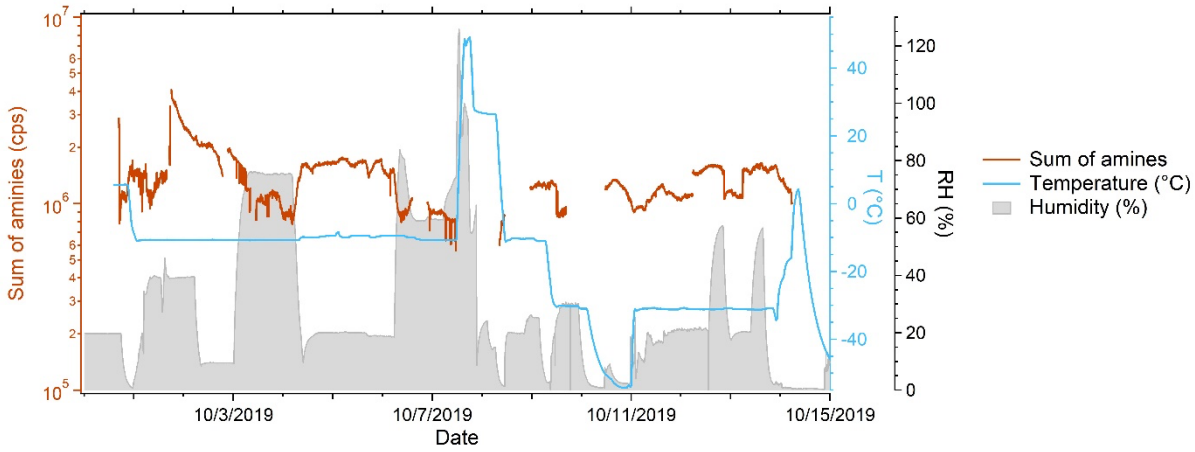

Figure S1 Time evolution of sum of the 13 amines used to normalize signal intensity. Temperature and humidity are also reported throughout the different experiments when the NH_4^+-Orbitrap was used.

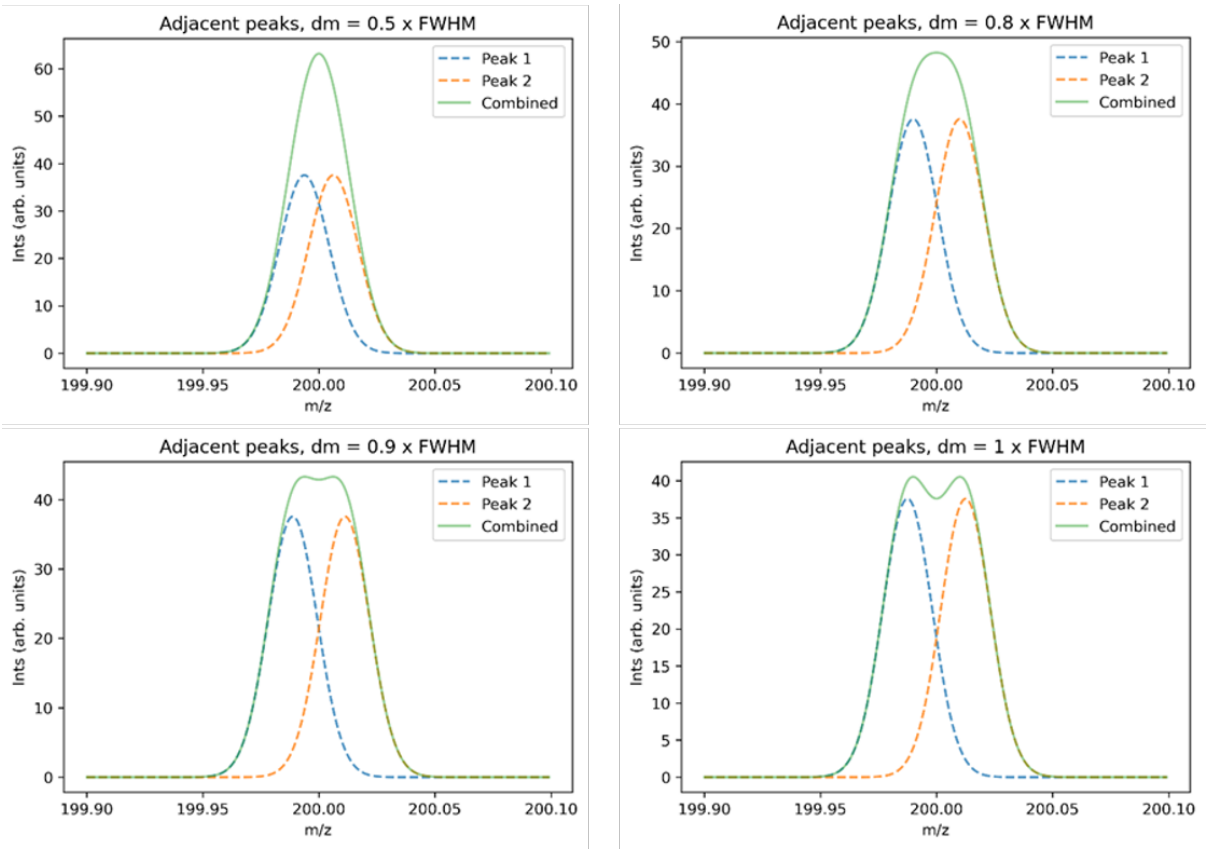

Figure S2 Simulated TOF spectra of overlapping peaks of equal intensity near m/Q 200 assuming a mass resolving power of 8,000, somewhere between that of a Tofwerk HTOF ("high-resolution time-of-flight') and LTOF ("long high-resolution time-of-flight) mass spectrometers. Noise wasn't added to the data.

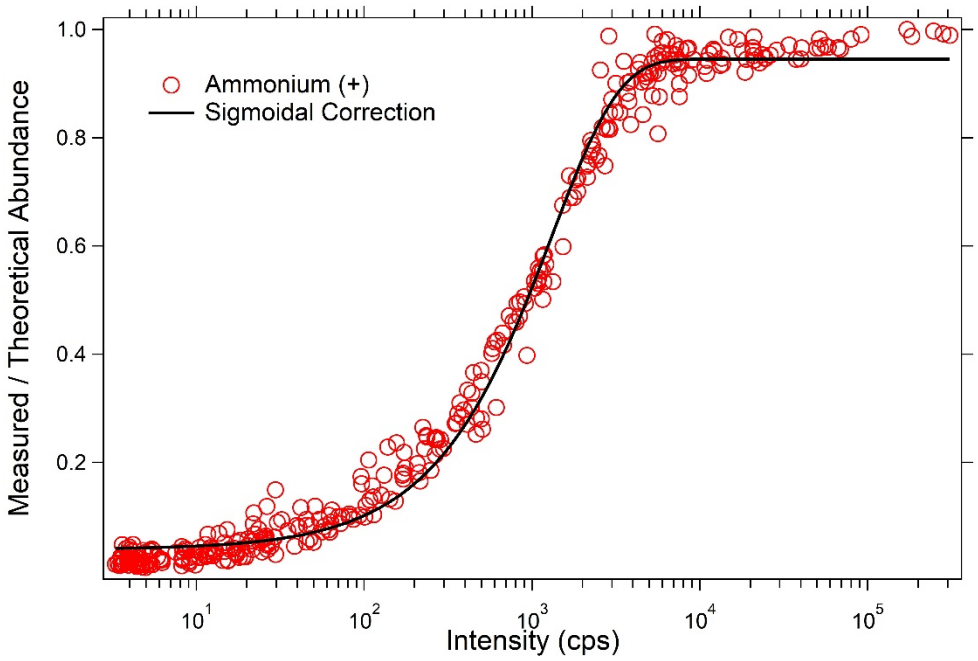

Figure S3 Linearity of the Orbitrap as a function of signal intensity measured with ammonium (NH_4^+) reagent ions. The black fit is the "sigmoidal correction function" based on a sigmoidal fitting algorithm.

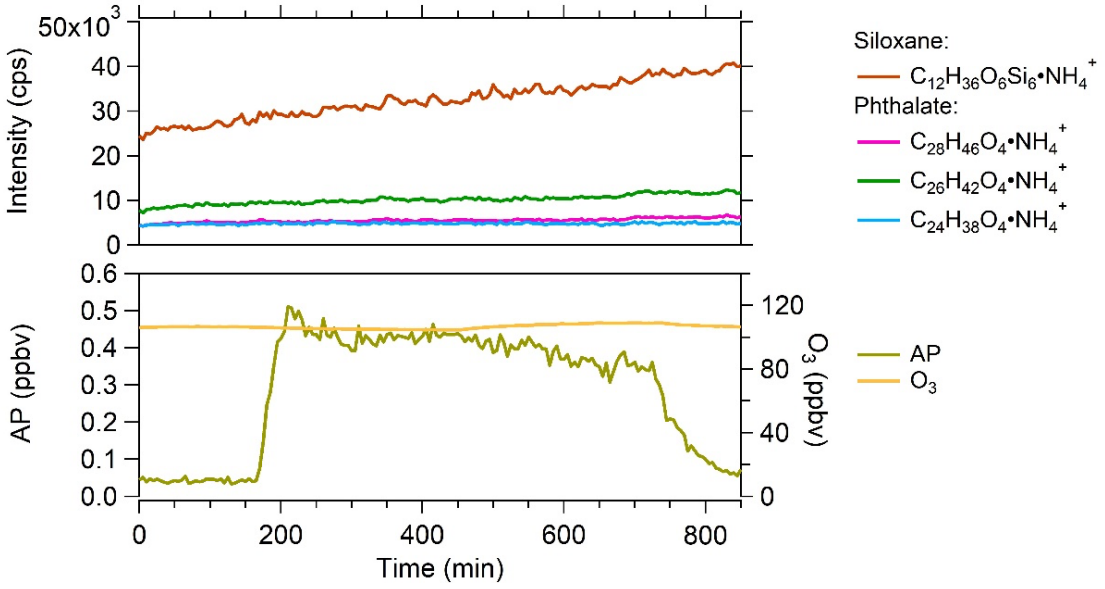

Figure S4 Constant time evolution of background ions showing the linearity of reagent ion NH_4^+. Siloxanes and phthalates clustered with NH_4^+ were not impacted by the addition of α-pinene, which means that the ionization technique remains linear under atmospheric relevant conditions. Run 2213: α-pinene oxidation products at -10 °C and 20% RH. α-pinene was ~0.41 ppbv and O_3 ~110 ppbv, NO_2 ~1.75 ppbv, NO ~0.12 ppbv and CO ~1000 ppbv.

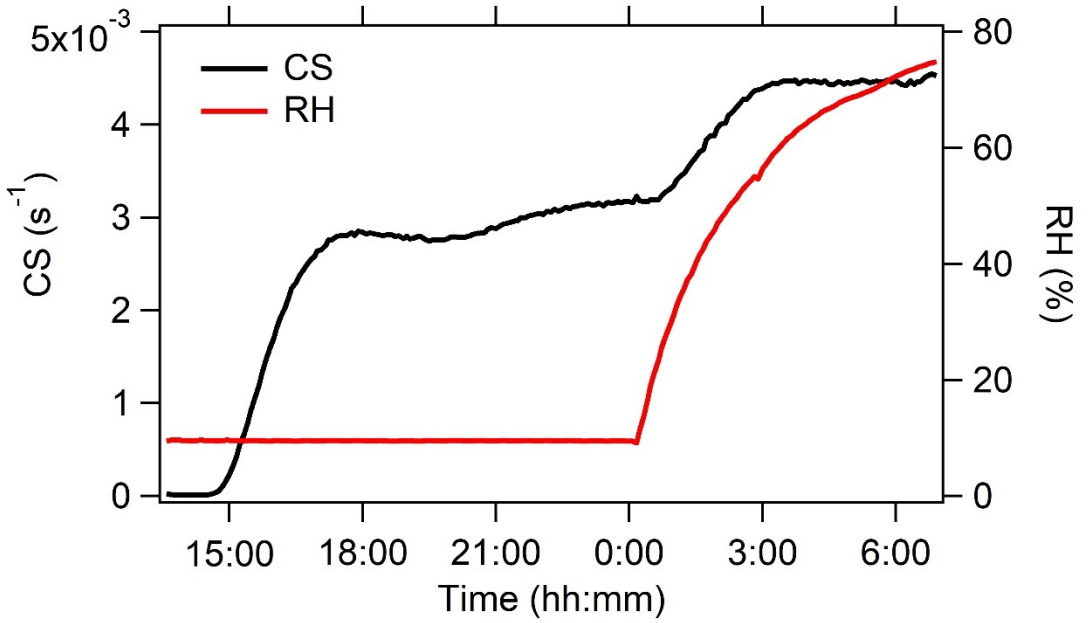

Figure S5 Time series of condensation sink (CS) where the RH is ramped up in run 2211.

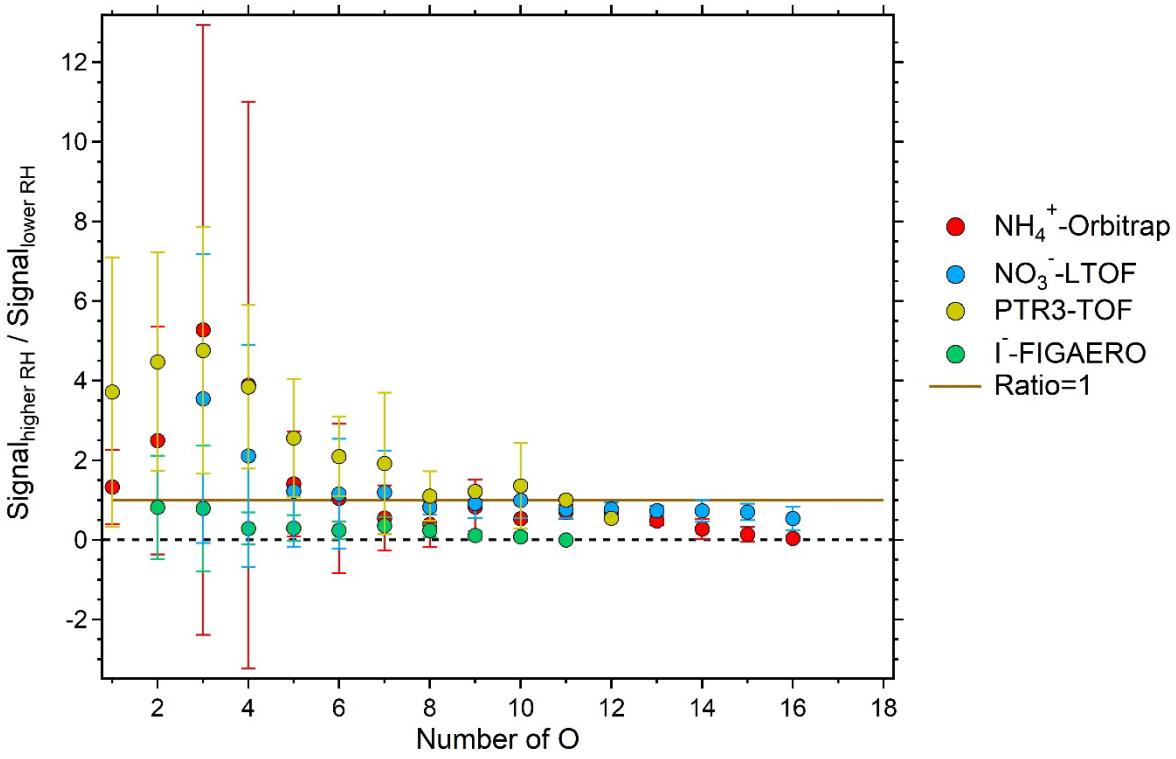

Figure S6: The relative humidity dependence of α-pinene oxidation products measured by four MS instruments as a function of number of oxygen atoms. All measured $C_{8\text{-}10}$ monomers and $C_{18\text{-}20}$ dimers are used to study an RH effect. The RH ramped from ~10% to ~80% in run 2211.