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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	Steady-state 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

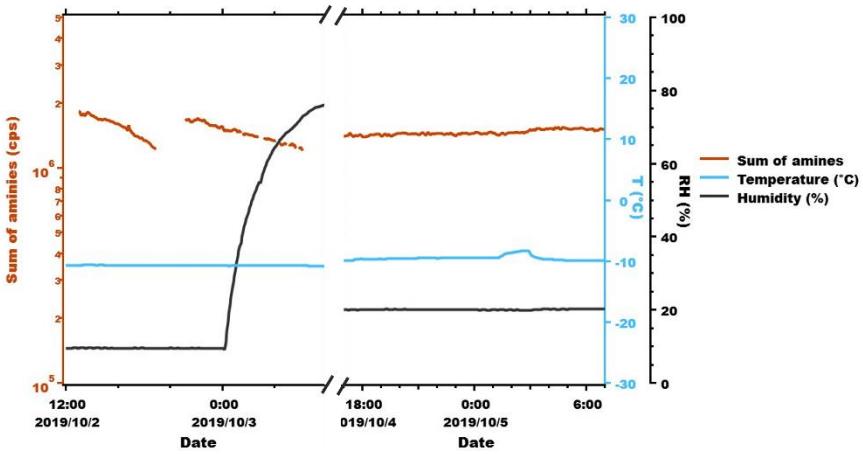

Figure S1 Time evolution of the sum of the 13 amines used to normalize signal intensity in runs 2211 and 2213. Temperature and humidity were also reported throughout the different experiments when the NH4+-Orbitrap was used.

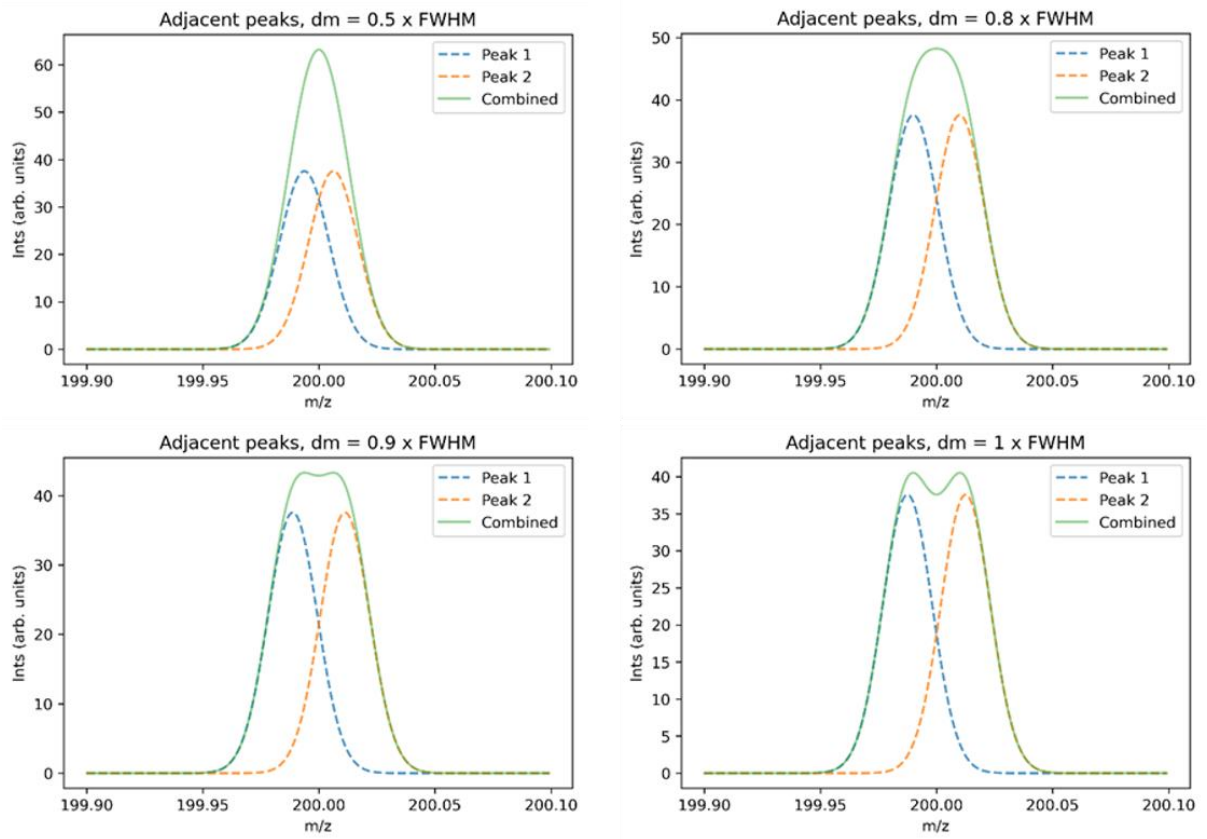

Figure S2 Simulated TOF spectra of overlapping peaks of equal intensity near m/Q 200 assuming a mass resolving power of 8,000, somewhere between that of a Tofwerk HTOF ("high-resolution time-of-flight') and LTOF ("long high-resolution time-of-flight) mass spectrometers. Noise wasn't added to the data.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

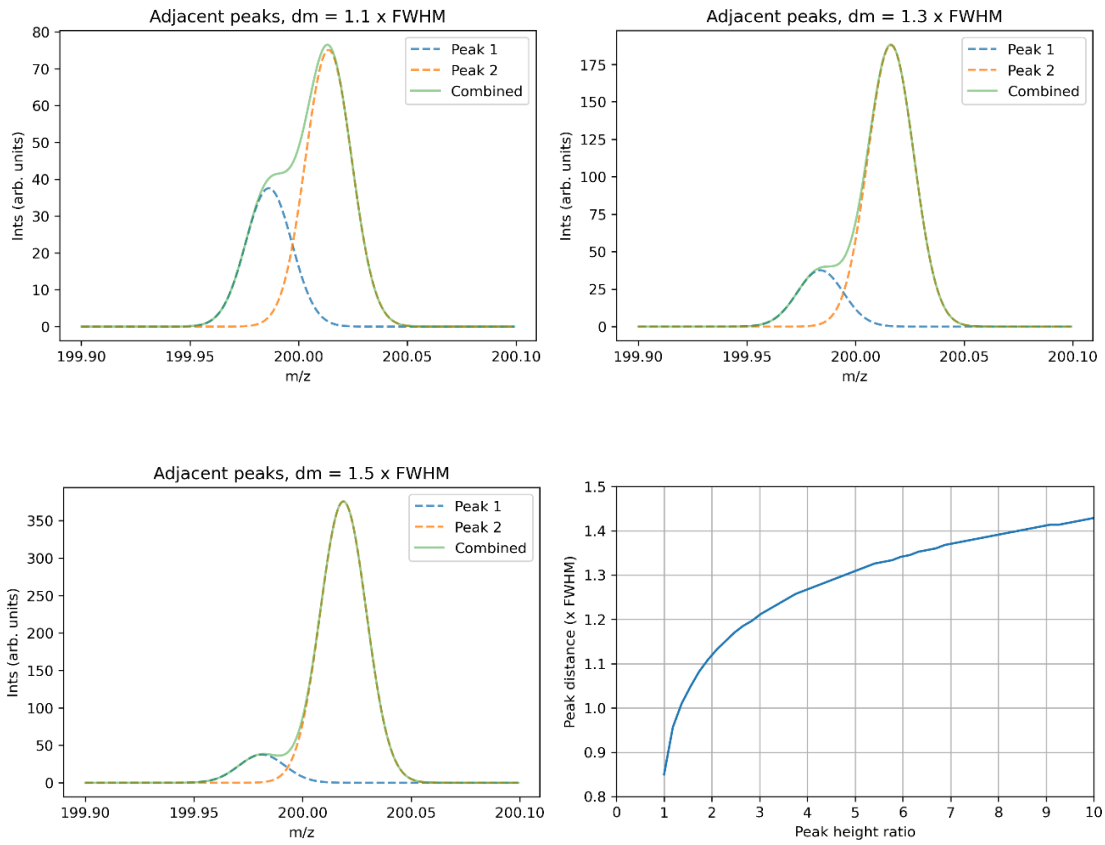

Figure S3 Simulated TOF spectra of overlapping peaks of equal intensity near *m/z* 200 assuming a mass resolving power of 8,000, somewhere between that of a Tofwerk HTOF ("high-resolution time-of-flight') and LTOF ("long high-resolution time-of-flight) mass spectrometers. The overlapping area represented a greater proportion of the peak area of the less intense peak. Noise wasn't added to the data. FWHM was the full width at half maximum and dm was the distance between two overlapping peaks. Peak height ratio represented the signal intensity ratio of overlapping peaks and peak distance referred to the ratio of dm to FWHM.

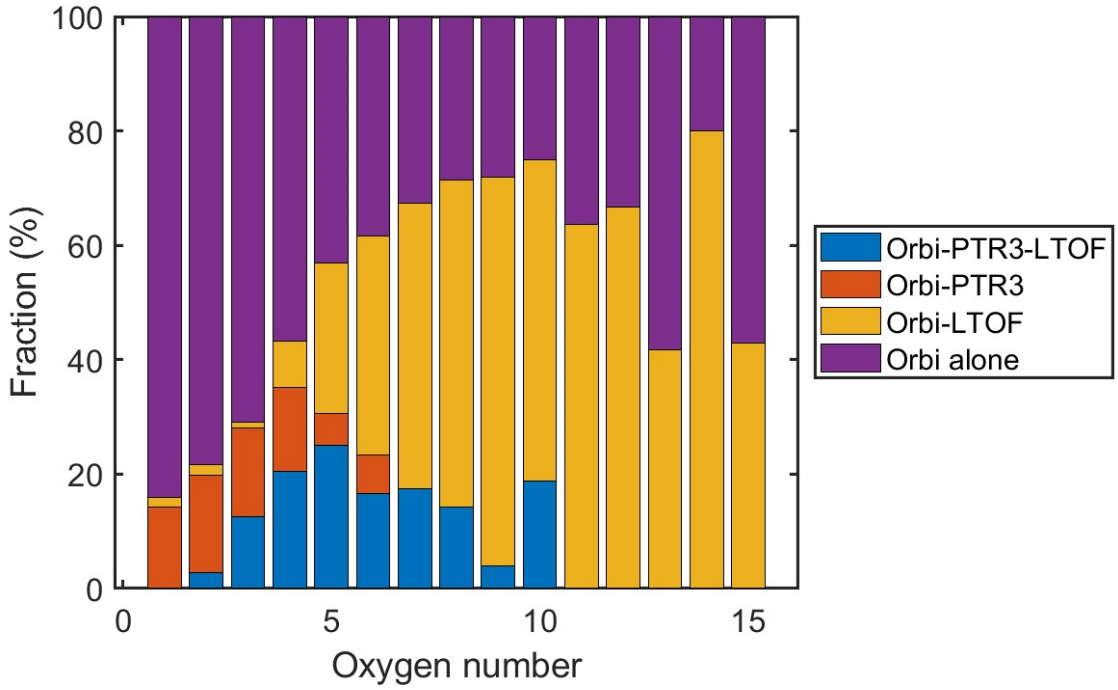

Figure S4 The fractions of co-detected OOMs with other instruments among those detected by NH_4^+-Orbitrap with the variation of oxygen number. Purple areas represent the OOMs only detected by NH_4^+-Orbitrap, which account for approximately 42%; yellow areas were OOMs co-detected by NH_4^+-Orbitrap and NO_3^--LTOF; red areas were OOMs co-detected by NH_4^+-Orbitrap and PTR3-TOF; and blue areas were OOMs co-detected by the three mass spectrometers.

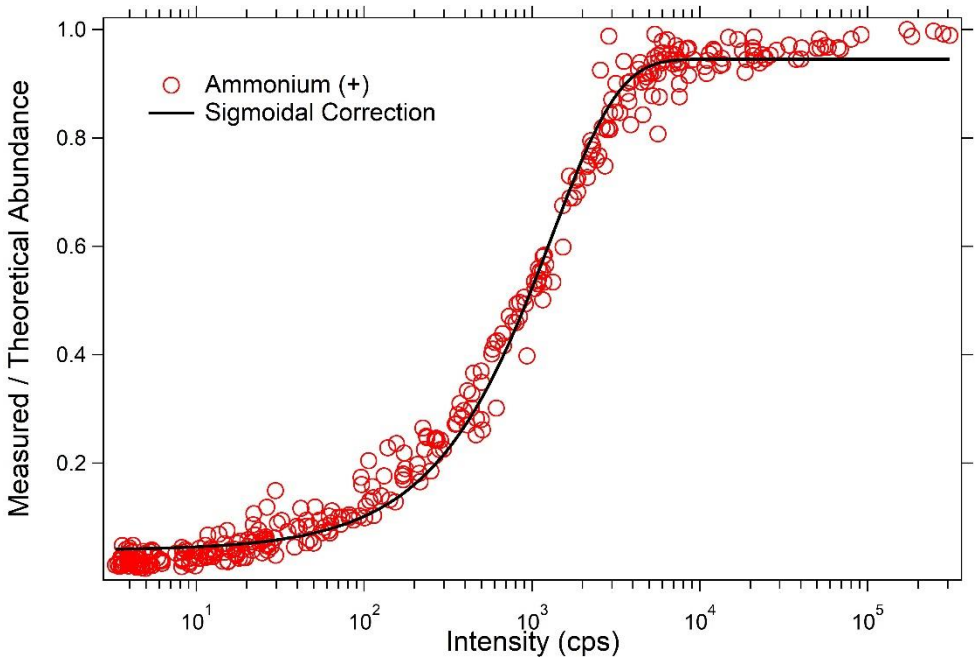

Figure S5 Linearity of the Orbitrap as a function of signal intensity measured with ammonium (NH_4^+) reagent ions. The black fit is the "sigmoidal correction function" based on a sigmoidal fitting algorithm.

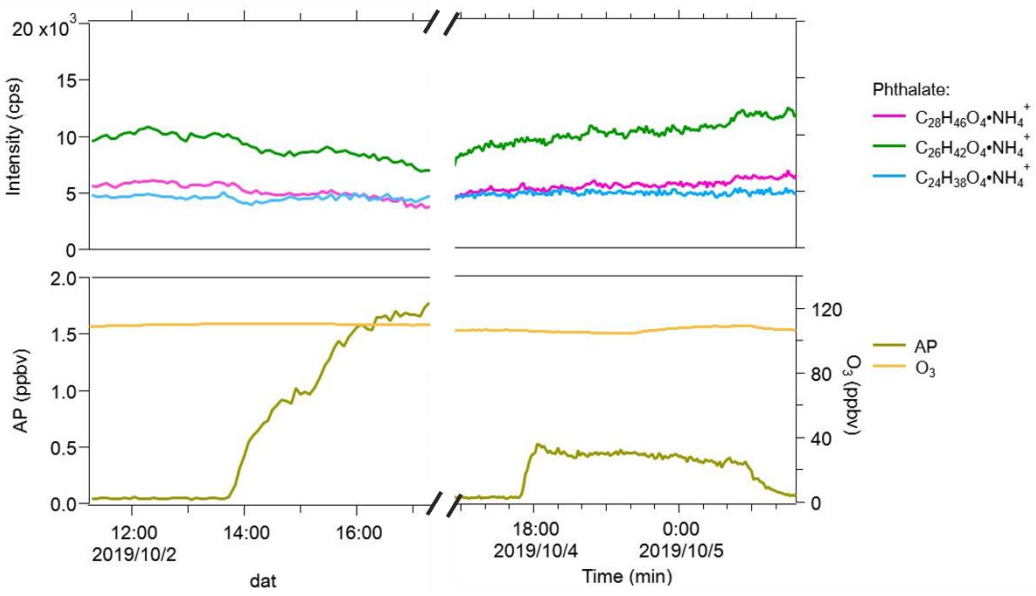

Figure S6 Constant time evolution of background ions showing the linearity of reagent ion NH_4^+ in run 2211 and run 2213. Siloxanes and phthalates clustered with NH_4^+ were not impacted by the addition of α-pinene, which means that the ionization technique remains linear under atmospheric relevant conditions.

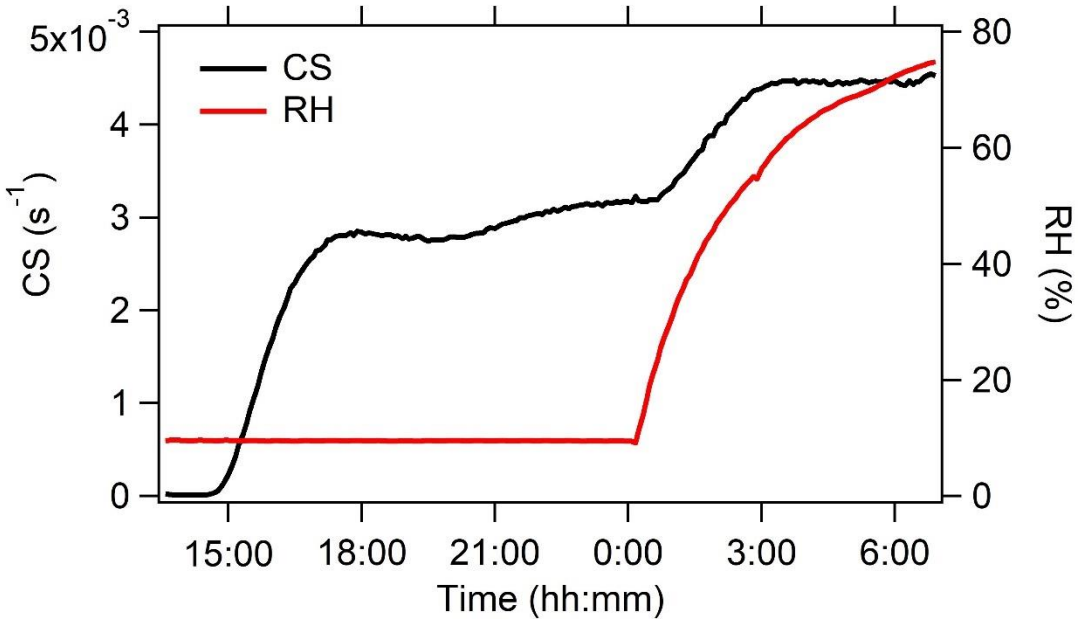

Figure S7 Time series of condensation sink (CS) where the RH is ramped up in run 2211.

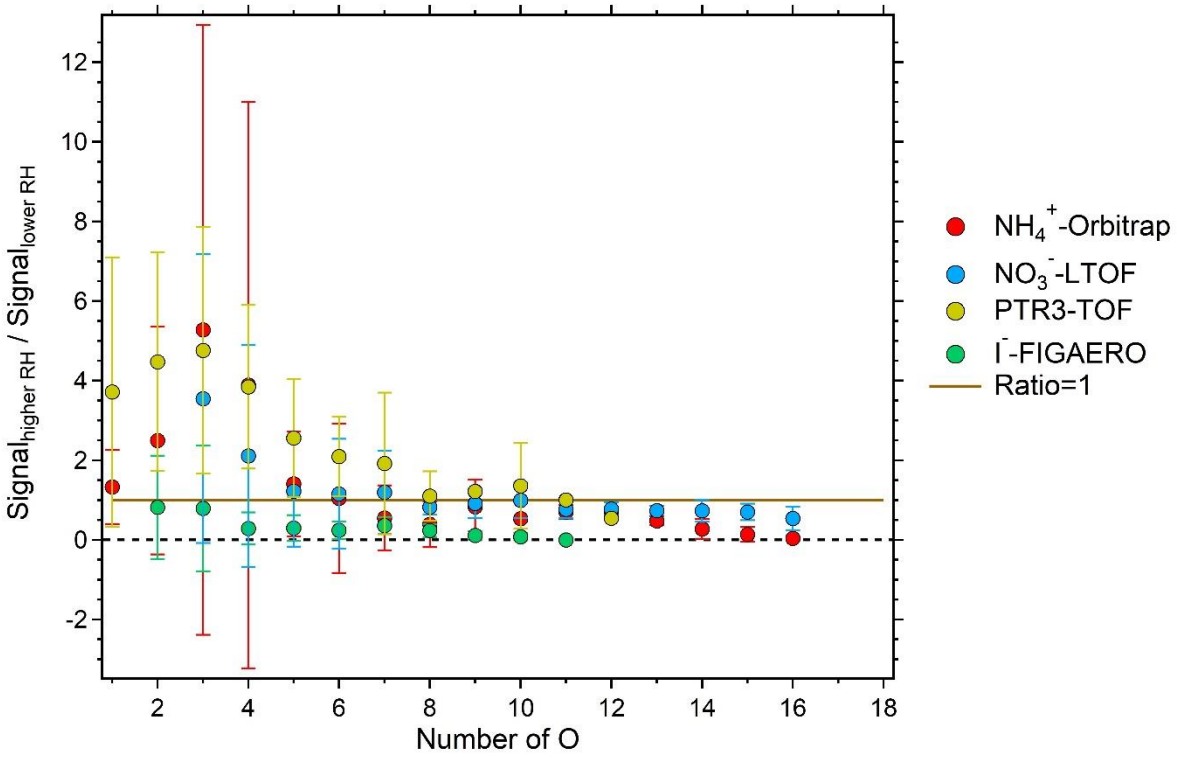

Figure S8 The relative humidity dependence of α-pinene oxidation products measured by four MS instruments as a function of number of oxygen atoms. All measured $C_{8\text{-}10}$ monomers and $C_{18\text{-}20}$ dimers are used to study an RH effect. The RH ramped from ~10% to ~80% in run 2211.