Supplement of Atmos. Meas. Tech., 19, 5491–5507, 2026
https://doi.org/10.5194/amt-19-5491-2026-supplement

Atmospheric Measurement Techniques
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EGU

Supplement of

Insufficient mass spectrometric detection of synthesized peroxy acids from α-pinene ozonolysis

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S1 Supplementary figures

Figures S1–S4 provide additional experimental results and supporting analyses referenced in the main manuscript.

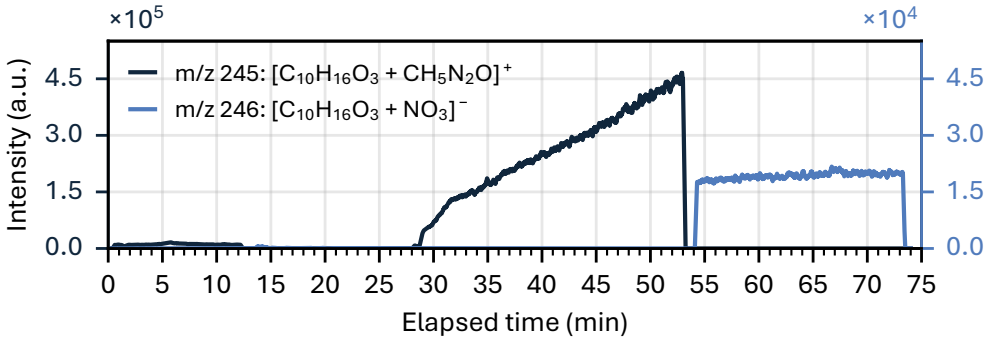

Figure S1: Extracted-ion chromatogram of pure pinonic acid (PA; $C_{10}H_{16}O_3$). The uronium adduct channel $[PA+CH_5N_2O]^+$ was recorded first; the abrupt change at approximately 54 min marks the switch to nitrate, after which the nitrate adduct channel $[PA+NO_3]^-$ is shown. Absolute intensities are displayed on separate axes. The pure PA signal continues to rise throughout the approximately 25 min uronium interval and retains a slightly increasing trend during the subsequent approximately 20 min nitrate interval, rather than reaching the rapid plateau observed for the paired peroxy pinonic acid (PPA) and PA signals in Fig. 5b.

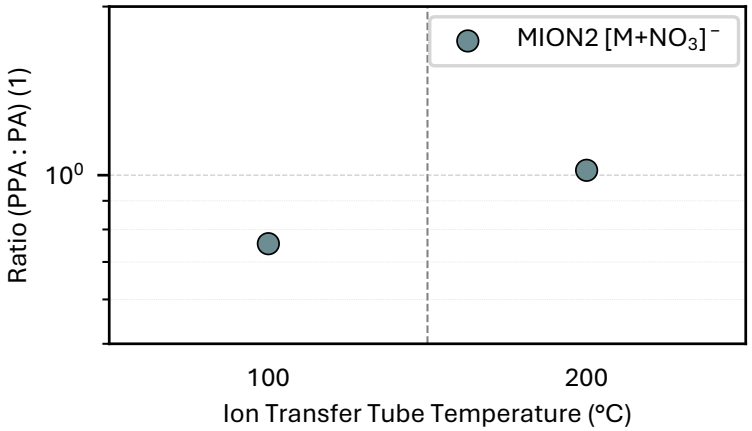

Figure S2: Nitrate adduct signal ratio of peroxy pinonic acid (PPA) to pinonic acid (PA) at ion transfer tube temperatures of 100 °C and 200 °C, calculated from 2 min averaged mass spectra. The ratio increases modestly with temperature from approximately 0.8 to approximately 1.0, but remains well below the NMR ratio of 4.7.

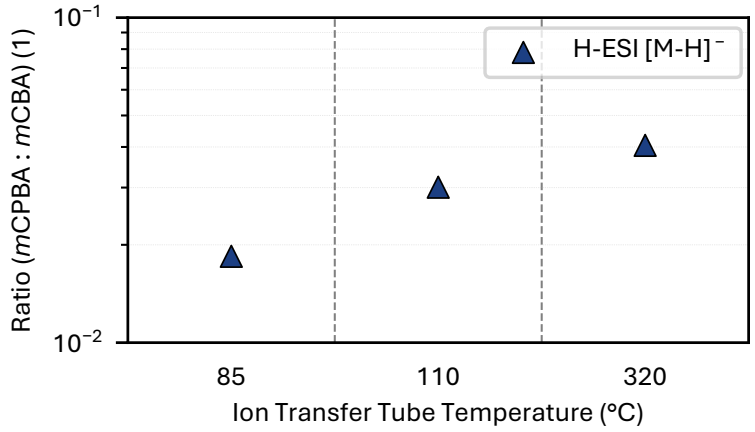

Figure S3: Signal ratio of deprotonated *meta*-chloroperoxybenzoic acid (*m*CPBA) to *meta*-chlorobenzoic acid (*m*CBA) measured with heated electrospray ionization (H-ESI) at ion transfer tube temperatures of 85 °C, 110 °C, and 320 °C, calculated from 30 s averaged mass spectra. The ratio increases modestly with temperature, but remains well below the approximate bulk *m*CPBA/*m*CBA ratio of 3.3.

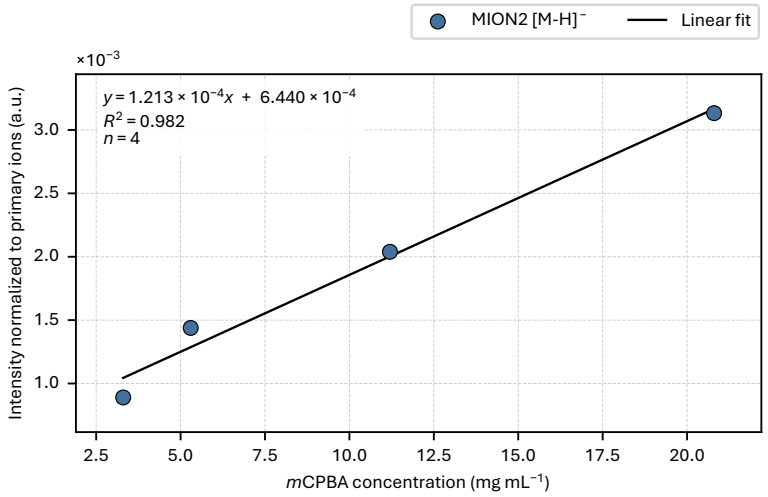

Figure S4: Nitrate mode response of the deprotonated *meta*-chloroperoxybenzoic acid (*m*CPBA) signal across four solution concentrations. Points represent 9 min mean intensities normalized to nitrate primary ions. The linear fit is $y = 1.213 \times 10^{-4}x + 6.440 \times 10^{-4}$ ($R^2 = 0.982$; $n = 4$). This control demonstrates a systematic low-intensity response for *m*CPBA in nitrate mode.