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Measurement of alkyl and multifunctional organic nitrates by proton-transfer-reaction mass spectrometry

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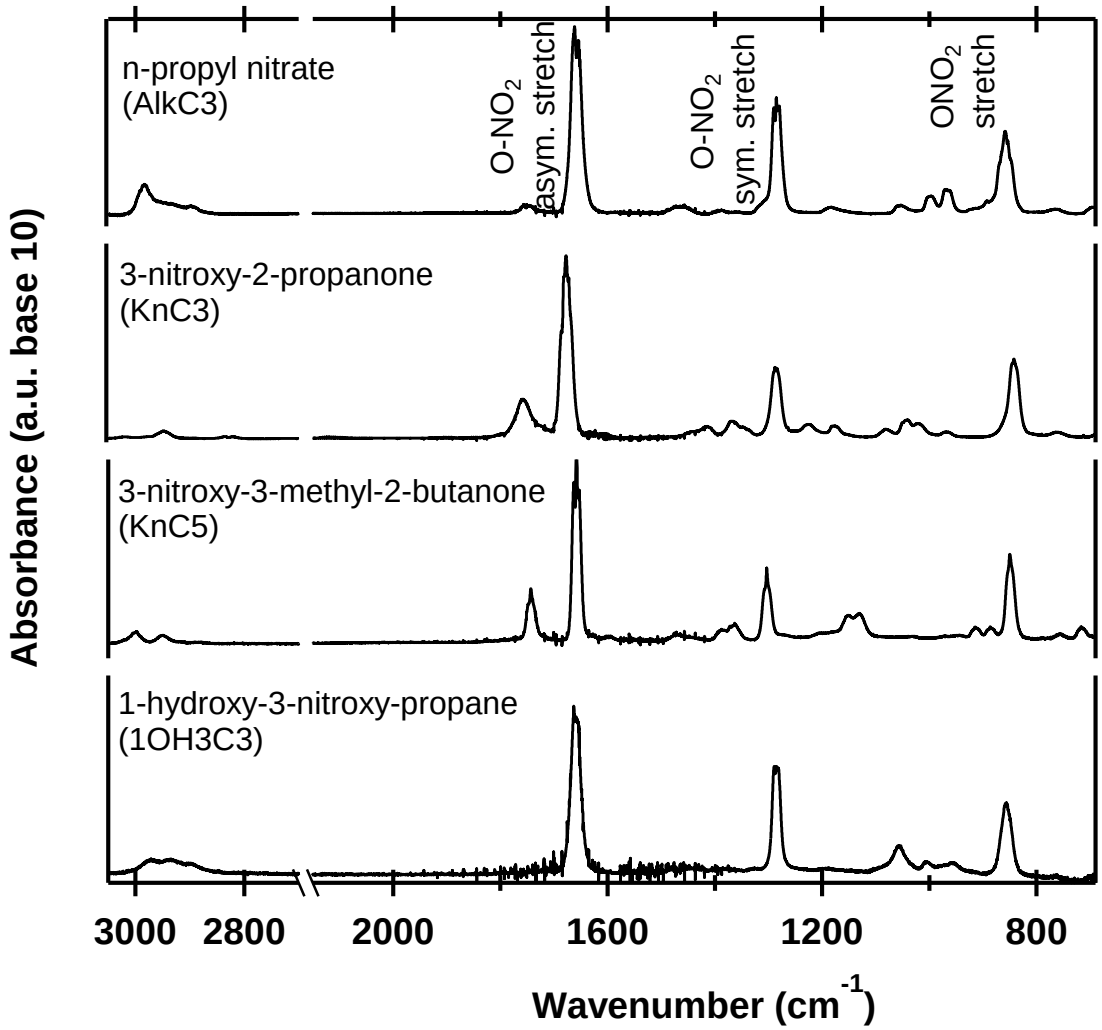

Figure S1. The FTIR gas phase absorbtion spectra of the synthesized organic nitrates (KnC3, KnC5, 1OH3C3) compared with a commercially available alkyl nitrate spectra (AlkC3).

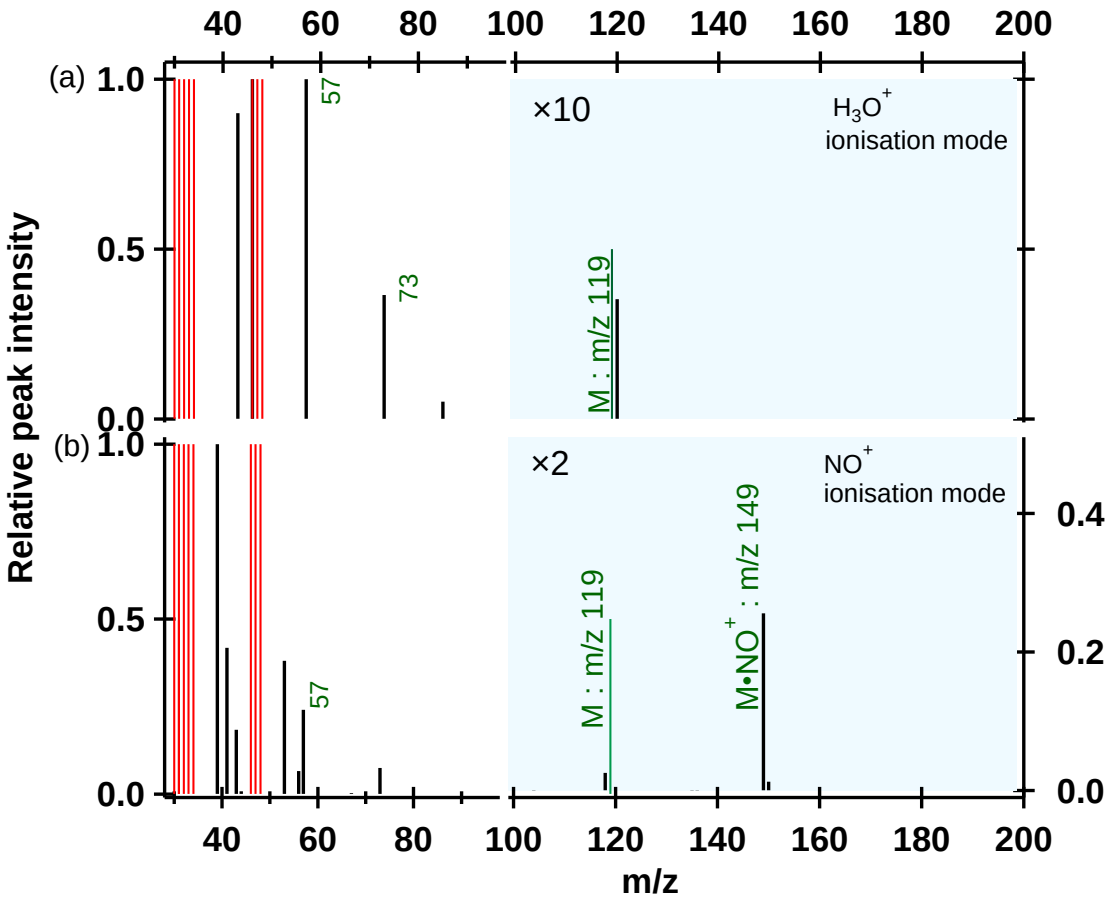

Figure S2. Recorded mass spectrum of protonated Alk*i*C4 (black bars) for E/N = 70 Td, corresponding to the highest sensibility for the protonated analyte signal detection (m/z 120) in absence of the RF device (a) and in the NO^+ ionization mode in presence of the RF (E/N* = 34 Td) (b). The green thin line represents the expected molecular ion of the analyte. The intense signals depicted by the red thin bars represent the ionizing and matrix analytes at m/z = 30 (NO^+) and 46 (NO_2^+) and their isotopic abundance signals at m/z = 31 and 47, 48 respectively. The signals corresponding to the water clusters $(H_3O^+(H_2O)_n$ at m/z 37 and 55 are systematically erased for simplification.

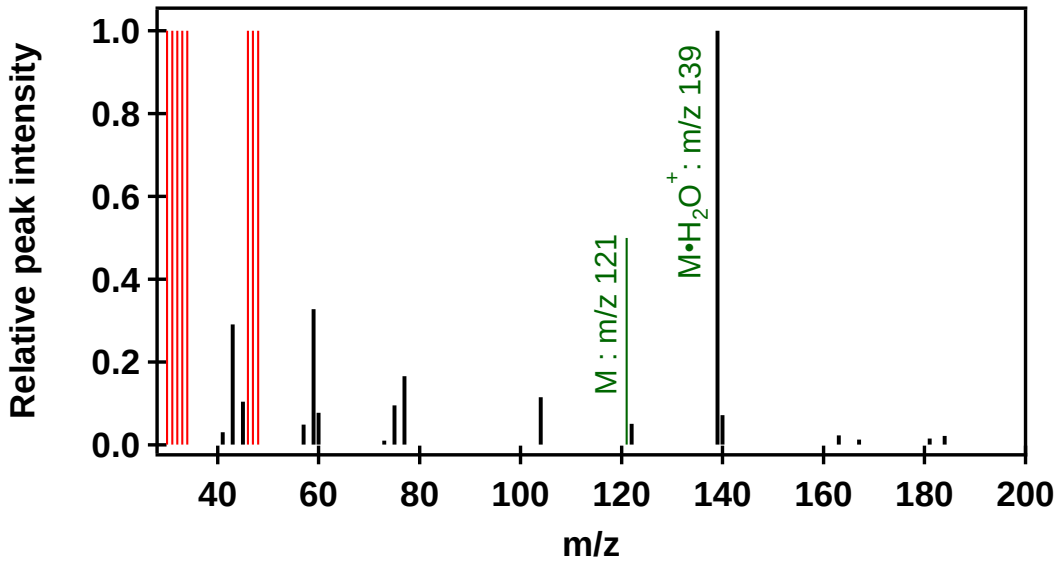

Figure S3. The recorded mass spectrum of 1OH3C3 (black bars) at the lowest extent of fragmentation (E/N* = 45 Td) in the H_3O^+ ionization mode under the influence of the RF mode.

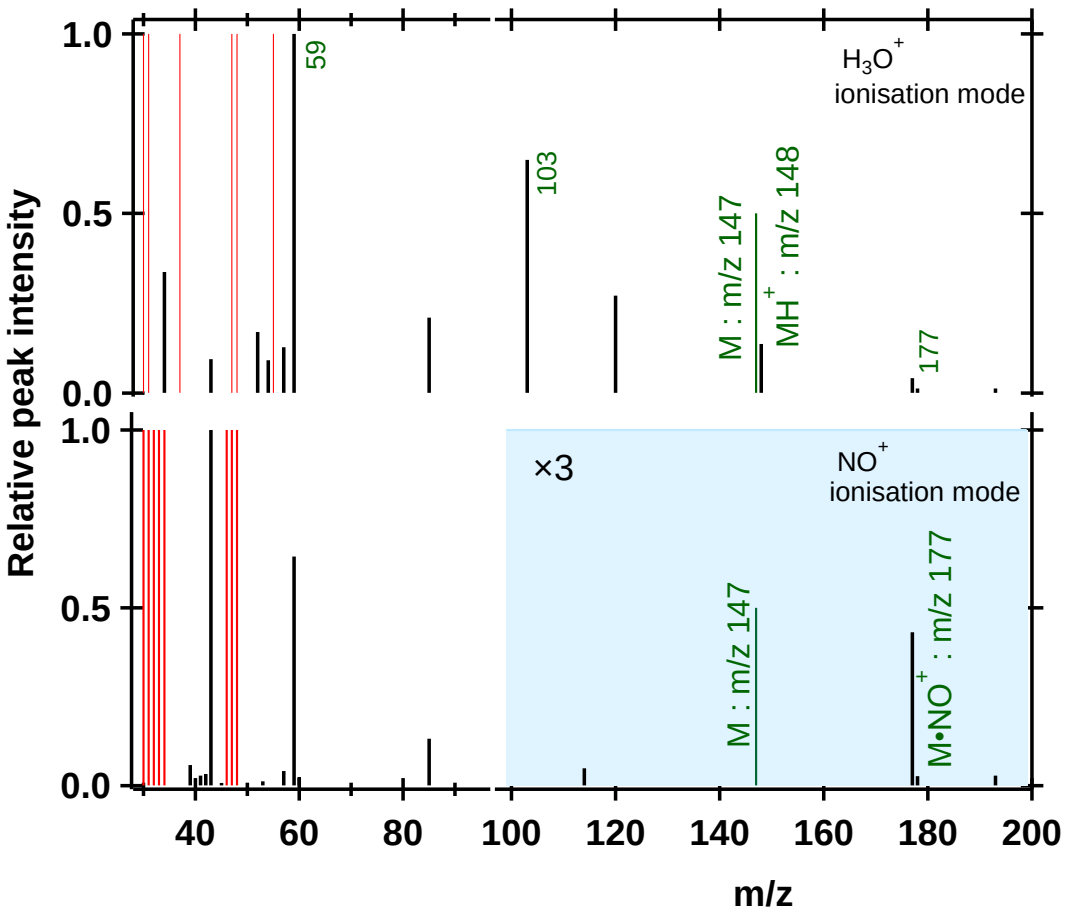

Figure S4. Recorded mass spectrum of protonated KnC5 (black bars) for E/N = 75 Td, corresponding to the highest sensibility for the protonated analyte signal detection (m/z 148) in absence of the RF device (a) and in the NO^+ ionization mode in presence of the RF (E/N* = 36 Td) (b). The green thin line represents the expected molecular ion of the analyte. The intense signals depicted by the red thin bars represent the ionizing and matrix analytes at m/z = 30 (NO^+) and 46 (NO_2^+) and their isotopic abundance signals at m/z = 31 and 47, 48 respectively. The signals corresponding to the water clusters $(H_3O^+(H_2O)_n$ at m/z 37 and 55 are systematically erased for simplification.

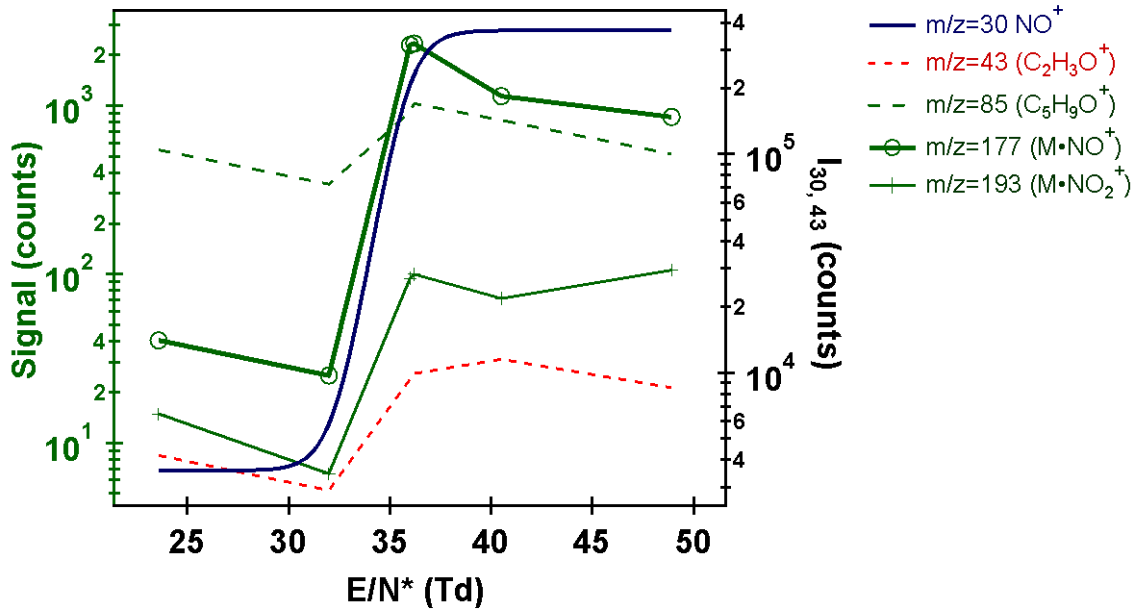

Figure S5. The RF mode behavior of typical NO^+ ionization signals of keto-nitrates (KnC5) under the E/N ratio influence (left axis). Typical distribution of the NO^+ ions and $C_2H_3O^+$ fragment into the given E/N interval (right axis).

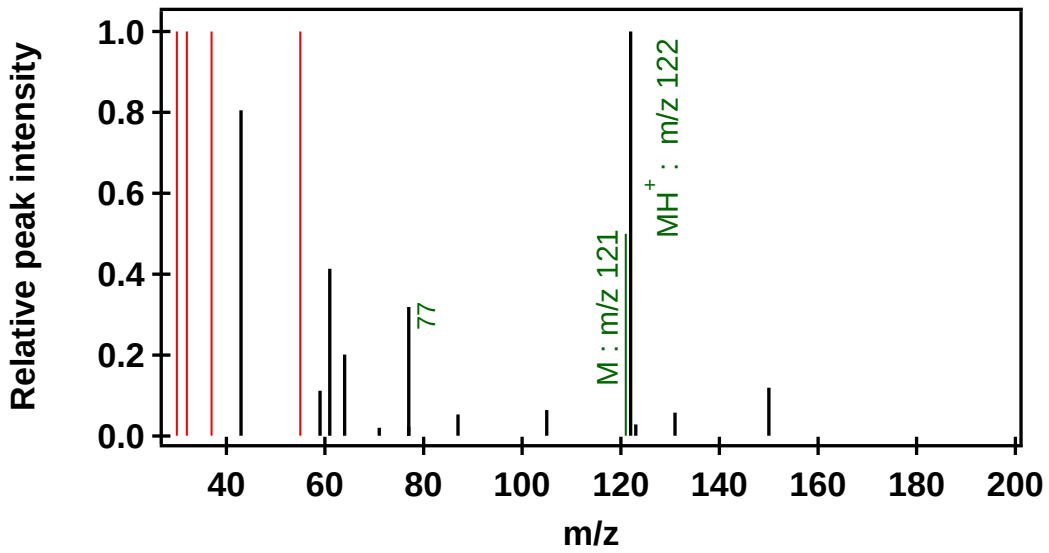

Figure S6. Recorded mass spectrum of protonated PAN (black bars) for E/N = 85 Td, corresponding to the highest sensibility of the m/z 122 signal detection.