



Measurements of highly oxidized multifunctional compounds from isoprene NO_3 reaction using bromide chemical ionization mass spectrometry

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Highly oxidized multifunctional molecules (HOMs) play a significant role in aerosol formation. They are expected to be reactive and with low volatility, which makes their measurement challenging. In this study, a high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS) using bromide as primary reagent ion was deployed to measure HOMs. Calibration experiments were performed using salicylic acid ($\text{C}_7\text{H}_6\text{O}_3$) as a calibration compound. The limit of detection is 0.8 ppt for a 1 min integration measurement, and the measurement sensitivity is approximately 112 ± 20 cps ppt⁻¹. Experiments were performed using this instrument in the atmospheric simulation chamber SAPHIR (Simulation of Atmospheric PHotochemistry In a large Reaction Chamber) in Forschungszentrum Jülich to measure HOMs formed from oxidation of isoprene through reaction with nitrate radicals in August 2018. Perfluoropentanoic acid ($\text{C}_5\text{HF}_9\text{O}_2$) was used as an internal standard to check the stability of the instrument. In addition, the instrument performance was tested by comparison with more widely-used iodide chemical-ionization mass spectrometer. Both measurements show that C_5 nitrooxy hydroperoxide and dihydroxy nitrate ($\text{C}_5\text{H}_9\text{NO}_5$), C_5 hydroxy nitrate ($\text{C}_5\text{H}_9\text{NO}_4$), C_5 hydroxy hydroperoxy nitrate ($\text{C}_5\text{H}_9\text{NO}_6$), C_5 hydroxy carbonyl nitrate ($\text{C}_5\text{H}_7\text{NO}_5$) were the major oxidation products, and a linear correlation coefficient 0.85 was achieved between two datasets. The slopes of linear regression for most species varied from 0.76 to 2.0, which indicated a relatively good agreement of two instruments. All these facts demonstrate that bromide CIMS used in this study is a reliable instrument to measure HOMs. A preliminary comparison of the chemical box model simulated and observed HOMs concentrations will be presented.