Geophysical Research Abstracts
Vol. 19, EGU2017-5643, 2017
EGU General Assembly 2017

Assessing the sensitivity of benzene cluster cation chemical ionization mass spectrometry toward a wide array of biogenic volatile organic compounds

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Chemical ionization mass spectrometry is a real-time, sensitive and selective measurement technique for the detection of volatile organic compounds (VOCs). The benefits of CIMS technology make it highly suitable for field measurements that requires fast (10Hz and higher) response rates, such as the study of surface-atmosphere exchange processes by the eddy covariance method. The use of benzene cluster cations as a regent ion was previously demonstrated as a sensitive and selective method for the detection of select biogenic VOCs (e.g. isoprene, monoterpenes and sesquiterpenes) *[Kim et al., 2016; Leibrock and Huey, 2000]*. Quantitative analysis of atmospheric trace gases necessitates calibration for each analyte as a function of atmospheric conditions. We describe a custom designed calibration system, based on liquid evaporation, for determination of the sensitivity of the benzene-CIMS to a wide range of organic compounds at atmospherically relevant mixing ratios (<200 ppt). We report on the effect of atmospheric water vapor and oxygen concentrations on instrument response for isoprene and a wide range of monoterpenes and sesquiterpenes. To gain mechanistic insight into the ion-molecule reactions and the role of water vapor and oxygen, we compare our measured sensitivities with a computational analysis of the charge distribution between the analyte, reagent ion and water molecules in the gas phase. These parameters provide insight on the ionization mechanism and provide parameters for quantification of organic molecules measured during field campaigns.

References

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