A Chemical Ionization Mass Spectrometer Utilizing Ammonium Ions for Measurements of Organic Compounds in the Atmosphere

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Introduction

We need more analytical techniques to unravel the complex mixture of atmospheric species. Here, we explore the measurement capability of a NH₄⁺ CIMS towards atmospheric organic compounds.

Kinetic Modeling of the Ion Distribution

- Mij represents H⁺(NH₃)(H₂O)
- The distribution of reagent ions is controlled by the FIMR E/N, Pressure, Temperature, and the ratio of NH₃/H₂O.

Instrument Sensitivity

- NH₄⁺H₂O + R -> NH₄⁺R + H₂O
- The dependence of sensitivities on the ratio of mz54/mz55, which is a function of NH₃/H₂O ratio.

Products Distribution

- Besides the parent ion (NH₄⁺R), other product ions are produced.

Parameterize the Sensitivity

- The dependence of corrected sensitivities on the kinetic energy of the analyte ions.

Field Measurements

- NH₄⁺H₂O is sensitive to a wide range of oxygenated organic compounds.

Conclusions

- NH₄⁺ is a versatile reagent ion for measurements of a wide range of oxygenated organic compounds.
- The instrument sensitivities and products distribution are strongly dependent on the instrument conditions.