Assigning Structures to Ions in Mass Spectrometry

John L. Holmes, Christiane Aubry, Paul M. Mayer

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Assigning Structures to Ions in Mass Spectrometry John L. Holmes, Christiane Aubry, Paul M. Mayer Summarizing our present knowledge of the structures and chemistry of small organic cations in the gas phase, Assigning Structures to Ions in Mass Spectrometry presents the methods necessary for determining gas-phase ion structures. It is a comprehensive resource of background material that is essential for the interpretation and understanding of organic mass spectra.

Following a historical introduction of chief discoveries, the book surveys current experimental methods for ion production and separation as well as those designed to reveal qualitative and quantitative aspects of gas-phase ions. It also examines the computational chemistry and theoretical calculations that provide complementary thermochemical, structural, and mechanistic information. Five selected case studies illustrate specific challenges associated with ion structure assignment and thermochemical problems. The last major section of the book contains the data for describing or identifying all ions containing C alone and C with H, O, N, S, P, halogens, and small organic cations.

Presenting material written by leading researchers in the field, Assigning Structures to Ions in Mass Spectrometry underscores the importance of understanding the behavior of small organic ions and gas-phase ion chemistry for making new ion structure assignments

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