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ION/ION REACTIONS IN THE PAUL TRAP: FUNDAMENTAL AND APPLIED CONSIDERATIONS FOR BIOPOLYMER ANALYSIS

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Gaseous bio-ions have exhibited rich chemistry including reaction phenomenologies such as proton transfer, hydrogen/deuterium exchange, nucleophilic substitution, electron transfer, clustering, and, of course, unimolecular decomposition. The latter reaction class is used routinely in bioanalytical applications of mass spectrometry, including applications of ion trap mass spectrometry. This presentation focuses on bi-molecular reactions involving ions derived from the analyte molecule of interest and an oppositely charged reagent species.

Particular emphasis in this talk is placed on the reactions of multiply-charged bio-ions with singly-charged ions of opposite polarity. The capability for such ion/ion reactions to manipulate bio-ion charge states can play an important role in several bioanalytical applications of interest. The focus of this presentation is on the use of charge state manipulation via ion/ion chemistry for the analysis of polymer mixtures, primarily polypeptide mixtures. The desired characteristics of the singly-charged reagent will be discussed along with implications of the kinetics of ion/ion reactions for bioanalysis with data presented to illustrate each point. Several polypeptide mixtures of known composition have been studied along with the electrospray behavior of each individual component observed in the absence of the other components. These studies provide useful insights into the extent to which the direct mixture analysis capabilities of electrospray can be expanded by the use of gaseous ion/ion chemistry. The talk is intended to appeal to an audience with interests in instrumentation, physical chemistry, analytical chemistry, ion chemistry, and protein identification.