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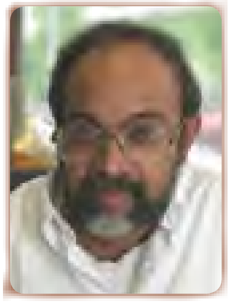

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Where is the charge located in multifunctional gaseous ions? A survey by ion mobility mass spectrometry

The preferred charge sites of protonated or deprotonated molecules in the gas phase has been a topic of extensive research. In fact, the exact location of the initial charge site of the precursor ion is requisite that should be addressed before any pragmatic interpretation of a fragmentation spectrum is attempted. Although the challenge appears seemingly simple, in reality it is not at all a trivial problem. One often assumes that the charge location can be easily predicted by knowing the gas-phase acidity or basicity of various groups present in a poly-functional molecule. However, in reality this is a very challenging problem because generalizations valid for solution-based chemistry cannot be extended directly to gas-phase phenomena. For example, there is sufficient experimental evidence to demonstrate that deprotonated p-hydroxybenzoic acid exists in gas phase as a mixture of carboxylate and phenoxide forms. Analogously, protonated aniline exists as mixture of nitrogen- or ring-protonated forms. Ion-mobility mass spectrometry (IM-MS) provides a way to determine relative population ratios of protomers or de-protomers that coexist under mass spectrometric ion generation conditions. Employing IM-MS separation, we demonstrate that mass spectrometric source conditions used for gas-phase ion generation play an important role on the relative ratios of isomeric protomers and de-protomers that coexist under a specific set of experimental conditions.

Biography

Athula Attygalle is a Professor at Stevens Institute of Technology, USA. He became the Director at Cornell University in 1991. After 12 years, he became a Professor at Stevens Institute of Technology in Hoboken, in 2001. He has published over 200 papers in reputed journals and holds five US patents

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