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Foreword

Gas phase ion chemistry: A fruitful playground for the interplay between experiment and theory

The use of theoretical methods as a research tool in all areas of chemistry has become increasingly important throughout the past decades. There are now well-established, reliable computational strategies based on solid theoretical methods that are often irreplaceable partners to experimental techniques. Theoretical calculations provide quantitative information on molecules and their interactions that are often difficult to determine experimentally. In addition, theory often provides detailed, fundamental understandings of molecular processes that are very hard and sometimes even impossible to obtain by experimental investigations alone. The most visible documentation of the importance of computational methods for all branches of chemistry is the award of the 1998 Noble Prize in chemistry to two exceptional scientists of this genre, John Pople and Walter Kohn. All this is probably best summarized in the following statement from the background information on this Nobel Prize: "Chemistry is no longer a purely experimental science."

Computational methods are particularly well suited for the treatment of isolated molecules where no perturbations due to the environment, such as solvent or crystal packing effects, need to be taken into account. It therefore comes as no surprise that the study of the structure, energetics, and reaction dynamics of gas-phase ions (including clusters and large molecules) represents an area of research where the synergism between sophisticated experiments and state-of-the-art theoretical and computational investigations has been particularly fruitful. This traditionally strong interaction between computational chemists and mass spectrometrists is reflected in the *International Journal of Mass Spectrometry* and other publications that have been important platforms for presenting computational or combined experimental/computational studies.

To provide an overview of the current state of the art in computational chemistry and its implications for gas-phase ion chemistry, the editors of the *International Journal of Mass Spectrometry* suggested devoting a special issue to various theoretical and computational aspects related to gas-phase ions. When we were asked to act as guest editors for this special issue we happily agreed, because both of us not only have a strong affinity for theoretical applications in gas-phase ion chemistry, but also feel that such a collection of contributions covering a wide range of different applications and methods will also serve as a valuable first orientation for newcomers to the field. This view was shared by many colleagues and we were able to compile a list of experts who accepted our invitation to contribute to this collection of computational papers. The 28 articles contained in this special issue cover a broad range of topics including highly accurate ab initio investigations on small model systems, studies on larger systems including clusters, contributions dealing with dynamical aspects of reactions and processes, etc. Many of the contributions are characterized by strong interaction with experiments or even include experimental

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studies, underlining the synergistic and fruitful interplay between theory and experiment so typical for this particular field.

We would like to thank the editors of the *International Journal of Mass Spectrometry*, in particular Mike Bowers and Helmut Schwarz for initiating this project. We owe a big thank you to all those who contributed to this special issue, not only for the high quality of the manuscripts but also for the timeliness in submissions and making revisions. In the same vein we would also like to thank the many anonymous reviewers for their prompt and thorough reports.

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