

PREFACE

Chemical reaction dynamics has been an important field in physical chemistry and chemical physics research during the last few decades. This field of research has provided crucial support for atmospheric chemistry, interstellar chemistry as well as combustion chemistry. The development in this field has also greatly enhanced our understanding of the nature of bimolecular and unimolecular chemical reactions, and intermolecular and intramolecular energy transfer processes. Even though this field of research reached relative maturity in the 1980s, it has made tremendous progress during the last decade or so. This is largely due to the development of many new and state-of-the-art experimental and theoretical techniques during that period. In view of these significant developments, it is beneficial to all of us that these developments be presented in a review volume to provide both graduate students and experts in the field a detailed picture of the current status of the advanced experimental and theoretical researches in chemical reaction dynamics. This review volume, published in two parts, is dedicated to the recent advances, both theoretical and experimental, in chemical reaction dynamics. All chapters in this volume are written by world experts in these special topics.

Experimentally, many new techniques have been developed in the last decade or so to study molecular reaction dynamics. For example, the velocity map imaging method for photochemistry and bimolecular reactions, the high resolution highly sensitive H-atom Rydberg tagging time-of-flight technique, the Doppler selected “core” mapping method, the significantly improved universal crossed molecular beam technique, coincident imaging method, etc. The application of VUV synchrotron radiation as well as soft ionization using traditional electron impact ionization in chemical dynamics has somewhat added species selectivity to the study of bimolecular as well as unimolecular reactions. The exciting development of femtosecond chemistry research has also provided us with the technique and the drive to look

at chemical reactions in the real time domain. These experimental methodologies are crucial for the advancement of our detailed understanding of the mechanisms of elementary chemical processes, complicated chemical reactions with multiple reaction pathways, photoionization/photodissociation processes, as well as intermolecular and intramolecular energy transfer processes.

On the theoretical front, the fast growing computing power and the development of sophisticated quantum, semiclassical and statistical methods in this research field allows us now to study complicated chemical processes quantitatively. The development of *ab initio* quantum chemistry has provided us with tools for obtaining accurate energetics as well as structural information on both small and large molecular systems. Based on *ab initio* calculations, accurate global potential energy surfaces can now be constructed for elementary chemical reactions for high-level dynamical studies. Dynamical calculations using exact full quantum methods as well as semiclassical methods can be carried out on these global potential surfaces. Combining these calculations with detailed analysis of the calculated results, mechanisms of elementary chemical reactions can now be studied in great detail. Interesting nonadiabatic dynamics involving interesting avoided crossings as well as conical intersections can now be studied using both quantum chemical and dynamical methods. Dynamics of larger systems such as large clusters and biomolecules can also be investigated. Furthermore, the interaction between experiment and theory is becoming stronger than ever. Experiment and theory can now be compared quantitatively in chemical dynamics even for very complicated systems. Such interactions have also enhanced our understanding in almost every front in this research field.

The 13 chapters in this first part describe a variety of frontiers in the chemical dynamics field. First experimentally, multiple channel dynamics using universal crossed beam methods is discussed in Chapter 1. Ion imaging studies of chemical dynamics is focused on in Chapter 2 by Chandler *et al.* Chapter 3 by Liu and Suits describes the dynamics of hydrogen atom abstraction from polyatomic molecules. Theoretically, Mebel writes in Chapter 4 on the *ab initio* potential energy surfaces of large reactions. Zhang *et al.* provides a detailed description on the theoretical dynamics treatment of complex reactions in Chapter 5. In Chapter 6, Schatz *et al.* gives a detailed account on the QCT studies of four-atom reactions. And in Chapter 7, Smith focuses on the topic of statistical rate theory for unimolecular and complex formation reactions. Truhlar *et al.* in Chapter 8 provides

an overall look on non-Born–Oppenheimer chemistry, while Nakamura *et al.* focuses on the semiclassical theory of nonadiabatic transition and tunneling in Chapter 9. Back to experimental studies, in Chapter 10, Neumark looks at the current status in the study of transition state spectroscopy, while Continetti and Hayden provide a detailed description on the elegant coincident imaging techniques in Chapter 11. Suzuki describes the application of time-resolved photoelectron spectroscopy and imaging in chemical dynamics in Chapter 12. In the last chapter (Chapter 13), Friedrich brings us the interesting topic of manipulating cold molecules with non-resonant field.

We appreciate very much the time and effort by all the authors in contributing to the individual chapters in their respective fields. We hope these contributions will provide a general view of current chemical dynamics research, and will be helpful to both experts and newcomers in the field. We are also grateful to the editors for their careful editing of this volume.

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