

FOREWORD

The 1990's have been characterized by great advances in physical chemistry and chemical physics and the resulting applications to molecular structure, the dynamics of molecules and their chemical reactions. The recently awarded Nobel prizes to our colleagues Harold Kroto, Robert Curl and Richard Smalley for the discovery of the C_{60} molecular structure document this fact for the larger public. At the same time there seems to be a world-wide trend to reduce the funding of the science called molecular spectroscopy which has been, and still is, the basis for a multitude of discoveries in our century. This molecular science encompasses such diverse fields as mass-spectroscopy, nuclear magnetic resonance spectroscopy, microwave and milli-meter wave spectroscopy, the application of Fourier transform methods in nuclear magnetic resonance, microwave and infrared high resolution spectroscopy, and the vast field of laser spectroscopy. These spectroscopic methods exploit almost the entire range of the electromagnetic spectrum up through the ultraviolet range. They have greatly enriched our knowledge concerning atoms and molecules and their reactions in forming clusters and new species under laboratory conditions, in planetary atmospheres and in interstellar clouds. The spectroscopic information and methods are the basis for all spectroscopic analysis techniques in chemistry, all remote sensing applications to the earth's atmosphere and to the stellar and interstellar medium, including molecular clouds, stars and planetary systems.

The present volume in the advanced series in physical chemistry contains contributions from nine internationally known laboratories of experts. The types of molecular systems considered range as far as high-resolution spectroscopy of transient molecules and rigorous quantum mechanical studies of radiative association in molecular ions. The interplay between original aspects of experimental high-resolution infrared spectroscopy and up-to-date *ab initio* theory is displayed beautifully. In order to exploit the information

revealed by the high quality of present day spectroscopic data, the quantum mechanical methods must provide correlation-free reduced forms of the Hamiltonians in order to obtain physically meaningful molecular parameters of high accuracy and precision. The spectroscopic constants adequate for the current requirements of the remote sensing community can only be derived by such advanced methods. The molecular Hamiltonian must also include the large amplitude motions in asymmetric top molecules that are relevant to observations in atmospheric physics and chemistry. The theoretical understanding of the formation of energy level clustering is elegantly shown for some basic triatomic molecules, an important aspect of highly excited states which has model value for larger species. Further contributions are concerned with hidden information in the spectra of symmetric top molecules and the importance of choosing the phase factors properly. Every transformation from one basis set to another produces transformation coefficients that depend on the phases of the wavefunctions defined. The extended molecular symmetry groups were derived for molecules consisting of two coaxial rotors, a challenging set of molecules that has tantalized spectroscopists for years. All these aspects of quantum theory and its application to molecular spectroscopy are discussed with respect to recently studied examples.

In summary this book contains an expert's tool kit for working in vibration-rotational spectroscopy and molecular dynamics that should be the basis for further developments and discoveries. The editor and contributor to this volume, Dr. Dusan Papousek, can be congratulated for putting such a timely issue together.

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