Molecular Quantum Mechanics

Third Edition

P. W. Atkins and R. S. Friedman

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methodologies with applications in virtually all branches of chemistry The increased sophistication accuracy and scope of the theory of chemistry are due to a large extent to the spectacular development of quantum chemistry and in this book the authors have made a remarkable effort to provide a modern account of the field From the Foreword by Paul Mezey University of Saskatchewan Quantum Chemistry Fundamentals to Applications develops quantum chemistry all the way from the fundamentals found in Part I through the applications that make up Part II The applications include molecular structure spectroscopy thermodynamics chemical reactions solvent effects and excited state chemistry The importance of this field is underscored by the fact that the 1998 Nobel Prize in Chemistry was awarded for the development of Quantum Chemistry

Molecular Physics and Elements of Quantum Chemistry Hermann Haken, Hans Christoph Wolf, 2013-03-09 This textbook is intended for use by students of physics physical chemistry and theoretical chemistry. The reader is presumed to have a basic knowledge of atomic and quantum physics at the level provided for example by the first few chapters in our book The Physics of Atoms and Quanta The student of physics will find here material which should be included in the basic education of every physicist This book should furthermore allow students to acquire an appreciation of the breadth and variety within the field of molecular physics and its future as a fascinating area of research For the student of chemistry the concepts introduced in this book will provide a theoretical framework for his or her field of study With the help of these concepts it is at least in principle possible to reduce the enormous body of empirical chemical knowledge to a few fundamental rules those of quantum mechanics In addition modem physical methods whose fundamentals are introduced here are becoming increasingly important in chemistry and now represent indispensable tools for the chemist As examples we might mention the structural analysis of complex organic compounds spectroscopic investigation of very rapid reaction processes or as a practical application the remote detection of pollutants in the air **Scientific and Technical Books** and Serials in Print ,1989 Molekülphysik und Quantenchemie Hermann Haken, Hans C. Wolf, 2013-03-09 Molek lphysik und Quantenchemie f hrt systematisch und leicht zug nglich in die Grundlagen der beiden Gebiete ein wie es zum Verst ndnis der physikalischen Eigenschaften von Molek len und der chemischen Bindung erforderlich ist Aufbauend auf Grundkenntnissen aus der Atom und Quantenphysik von den gleichen Autoren vermittelt es den Studenten der Physik der Physikalischen Chemie und der Theoretischen Chemie die experimentellen und theoretischen Grundlagen und deren Wechselwirkung Die vorliegende vierte Auflage wurde um wesentliche aktuelle Entwicklungen experimenteller Methoden und theoretischer Ans tze erweitert Ebenso ist ein neues Kapitel zu Einzelmolek len u Einzelmolek l Spektroskopie hinzugekommen 133 Aufgaben vervollst ndigen das Buch Die dazugeh rigen L sungen k nnen im Internet abgerufen werden

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