

QUANTUM CHEMISTRY & SPECTROSCOPY

THIRD EDITION



THOMAS ENGEL

Quantum Chemistry Spectroscopy

Thomas Engel



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Equilibrium Molecular Structures Jean Demaison, James E. Boggs, Attila G. Csaszar, 2016-04-19 Molecular structure is the most basic information about a substance determining most of its properties Determination of accurate structures is hampered in that every method applies its own definition of structure and thus results from different sources can yield significantly different results Sophisticated protocols exist to account for these

Physical Chemistry Thomas Engel, Philip Reid, Alex Angerhofer, 2018-01-16 Chapter 15 Computational chemistry was contributed by Warren Hehre CEO Wavefunction Inc Chapter 17 Nuclear magnetic resonance spectroscopy was contributed by Alex Angerhofer University of Florida

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quantum chemistry Quantum chemistry is applied to explain and predict molecular spectroscopy and the electronic structure of atoms and molecules In addition the text provides a practical guide to using molecular mechanics and electronic structure computations including ab initio semi empirical and density functional methods The use of electronic structure computations is a timely subject as its applications in both theoretical and experimental chemical research is increasingly prevalent This text is written in a format that fosters mastery of the subject both in competency in the mathematics and in obtaining a conceptual understanding of quantum mechanics The chemistry student's interest is maintained early on in the text where quantum mechanics is developed by applying it to molecular spectroscopy and through conceptual questions labeled as Chemical Connection Questions throughout the text labeled as Chemical Connection and Points of Further Understanding focus on conceptual understanding and consequences of quantum mechanics If an Instructor chooses these questions can be used as a basis for classroom discussion encouraging cooperative learning techniques This text provides a solid foundation from which students can readily build further knowledge of quantum chemistry in more advanced courses In cases where this is a final course in quantum chemistry this text provides the student not only with an appreciation of the importance of quantum mechanics to chemistry but also with a practical guide to using electronic structure computations

Advances in the Theory of Atomic and Molecular Systems Piotr Piecuch, Jean Maruani, Gerardo Delgado-Barrio, Stephen Wilson, 2009-09-30 Advances in the Theory of Atomic and Molecular Systems is a collection of contributions presenting recent theoretical and computational developments that provide new insights into the structure properties and behavior of a variety of atomic and molecular systems This volume subtitled Dynamics Spectroscopy Clusters and Nanostructures deals with the topics of Quantum Dynamics and Spectroscopy Complexes and Clusters and Nanostructures and Complex Systems This volume is an invaluable resource for faculty graduate students and researchers interested in theoretical and computational chemistry and physics physical chemistry and chemical physics molecular spectroscopy and related areas of science and engineering

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Molecular Physics and Elements of Quantum Chemistry Hermann Haken,Hans Christoph Wolf,2013-04-18 Since the publication of the first edition of this book there have been many important new developments in the field of molecular physics The new methods and results which are most significant for students are treated extensively in this second edition Among these are in particular single molecule spectroscopy and the field of molecular electronics which is in a stage of rapid development including the areas of electroluminescence and organic light emitting diodes In addition we have extended and corrected the earlier material in a number of places We have also included exercises in this new edition they will allow students to deepen their understanding and offer a basis for further individual study The complete solutions to the exercises can be found on the Internet under www.springeronline.com 3 540 40792 S We are grateful to Mr C D Bachem and Dr Th Schneider of the Springer Verlag for their continuous and very agreeable cooperation during the preparation of the book We thank our colleague Prof W D Brewer for his competent translation Stuttgart February 2004 H Haken H C Wolf Preface to the First Edition 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

Computational Molecular Spectroscopy Per Jensen,Philip R. Bunker,2000-11-02 This book describes the use of modern computational methods in predicting high resolution molecular spectra which allows the experimental spectroscopist to interpret and assign real spectra Offers a comprehensive treatment of modern computation techniques Provides a collection of material from different areas of theoretical chemistry and physics Bridges the gap between traditional quantum chemistry and experimental molecular spectroscopy

Quantum Mechanical Foundations of Molecular Spectroscopy Max Diem,2021-07-19 A concise textbook bridging quantum theory and spectroscopy Designed as a practical text Quantum Mechanical Foundations of Molecular Spectroscopy covers the quantum mechanical fundamentals of molecular spectroscopy from the view of a professional spectroscopist rather than a theoretician Written by a noted expert on the topic the book puts the emphasis on the relationship between spectroscopy and quantum mechanics and provides the background information and derivations of the subjects needed to understand spectroscopy including stationary energy states transitions between these states selection rules and symmetry The phenomenal growth of all forms of spectroscopy over the past eight decades has contributed enormously to our understanding of molecular structure and properties Today spectroscopy covers a broad field including the modern magnetic resonance techniques non linear laser and fiber based spectroscopy surface and surface enhanced spectroscopy pico and femtosecond time resolved spectroscopy and many more

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