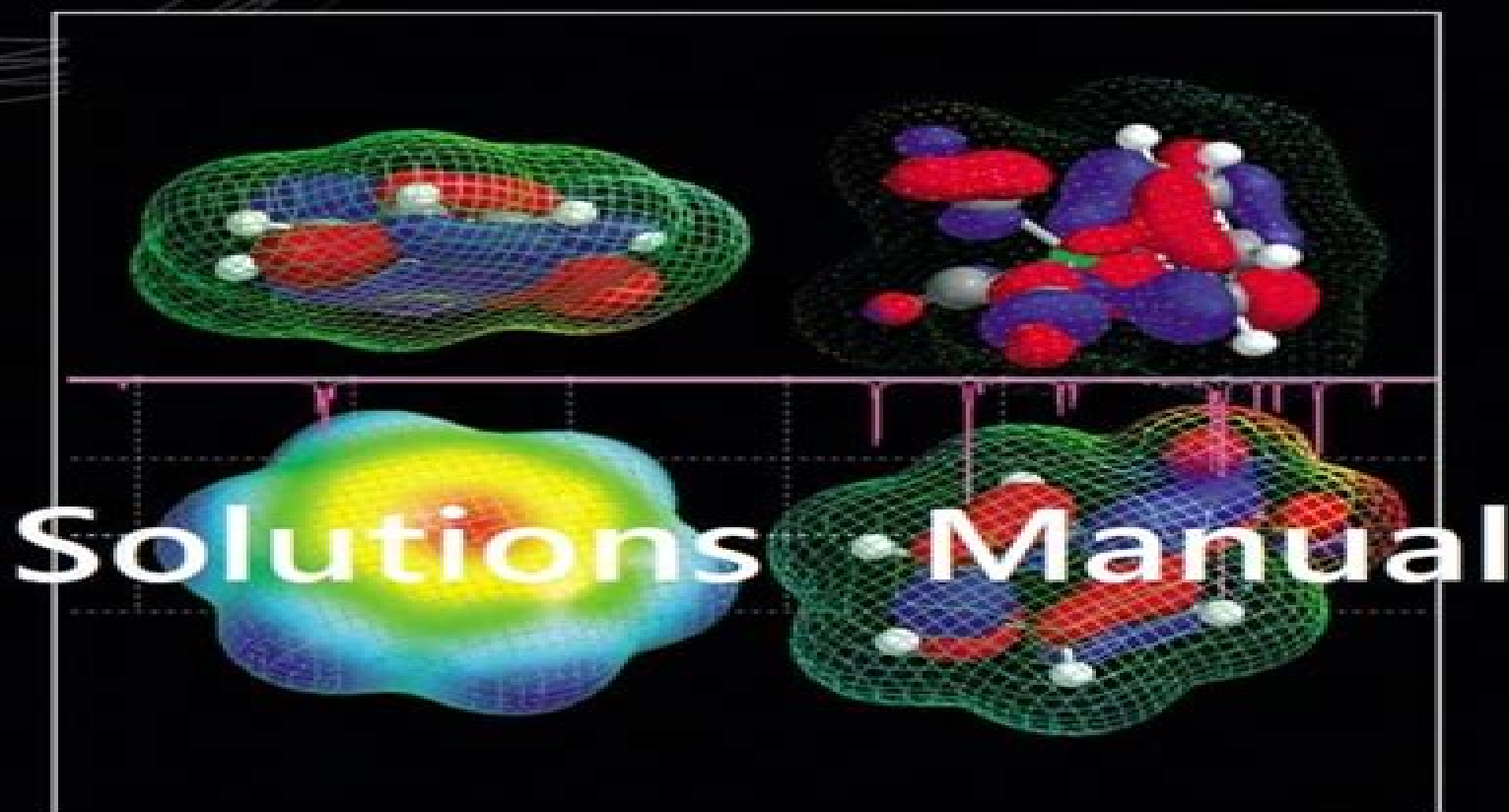


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BOOK JACKET **Quantum Chemistry** Ajit Thakkar, 2017-10-03 This book provides non specialists with a basic understanding of the underlying concepts of quantum chemistry It is both a text for second or third year undergraduates and a reference for researchers who need a quick introduction or refresher All chemists and many biochemists materials scientists engineers and physicists routinely use spectroscopic measurements and electronic structure computations in their work The emphasis of Quantum Chemistry on explaining ideas rather than enumerating facts or presenting procedural details makes this an excellent foundation text reference The keystone is laid in the first two chapters which deal with molecular symmetry and the postulates of quantum mechanics respectively Symmetry is woven through the narrative of the next three chapters dealing with simple models of translational rotational and vibrational motion that underlie molecular spectroscopy and statistical thermodynamics The next two chapters deal with the electronic structure of the hydrogen atom and hydrogen molecule ion respectively Having been armed with a basic knowledge of these prototypical systems the reader is ready to learn in the next chapter the fundamental ideas used to deal with the complexities of many electron atoms and molecules These somewhat abstract ideas are illustrated with the venerable Huckel model of planar hydrocarbons in the penultimate chapter The book concludes with an explanation of the bare minimum of technical choices that must be made to do meaningful electronic structure computations using quantum chemistry software packages **Books in Print**, 1991

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Annual ,1980 Student's Solutions Manual Thomas Engel,2010 **Modern Vibrational Spectroscopy and Micro-Spectroscopy** Max Diem,2015-08-17 Modern Vibrational Spectroscopy and Micro Spectroscopy Theory Instrumentation and Biomedical Applications unites the theory and background of conventional vibrational spectroscopy with the principles of microspectroscopy It starts with basic theory as it applies to small molecules and then expands it to include the large biomolecules which are the main topic of the book with an emphasis on practical experiments results analysis and medical and diagnostic applications This book is unique in that it addresses both the parent spectroscopy and the microspectroscopic aspects in one volume Part I covers the basic theory principles and instrumentation of classical vibrational infrared and Raman spectroscopy It is aimed at researchers with a background in chemistry and physics and is presented at the level suitable for first year graduate students The latter half of Part I is devoted to more novel subjects in vibrational spectroscopy such as resonance and non linear Raman effects vibrational optical activity time resolved spectroscopy and computational methods Thus Part 1 represents a short course into modern vibrational spectroscopy Part II is devoted in its entirety to applications of vibrational spectroscopic techniques to biophysical and bio structural research and the more recent extension of vibrational spectroscopy to microscopic data acquisition Vibrational microscopy or microspectroscopy has opened entirely new avenues toward applications in the biomedical sciences and has created new research fields collectively referred to as Spectral Cytopathology SCP and Spectral Histopathology SHP In order to fully exploit the information contained in the micro spectral datasets methods of multivariate analysis need to be employed These methods along with representative results of both SCP and SHP are presented and discussed in detail in Part II

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