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Principles and Applications of Quantum Chemistry offers clear and simple coverage based on the author's extensive teaching at advanced universities around the globe. Where needed, derivations are detailed in an easy-to-follow manner so that you will understand the physical and mathematical aspects of quantum chemistry and molecular electronic structure. Building on this foundation, this book then explores applications using illustrative examples to demonstrate the use of quantum chemical tools in research problems. Each chapter also uses innovative problems and bibliographic references to guide you and throughout the book chapters cover important advances in the field including Density functional theory (DFT) and time-dependent DFT (TD-DFT) characterization of chemical reactions, prediction of molecular geometry, molecular electrostatic potential, and quantum theory of atoms in molecules. Simplified mathematical content and derivations for reader understanding. Useful overview of advances in the field such as Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT). Accessible level for students and researchers interested in the use of quantum chemistry tools.

An Introduction to Physical Chemistry D. K. Chakrabarty, 2001. This book is intended for undergraduate students and may also be used for a first chemistry course. The emphasis is on the concepts of physical chemistry and how to obtain quantitative relations from the concepts. Representative problems are included at the end of every chapter. To reduce the bulk, the book avoids experimental details that should be covered in laboratory manuals. Some aspects such as wave mechanical model of the atom, molecular symmetry, chemical bonding, and solid state chemistry that are inadequately covered by most text books at this level are discussed in detail to give flavour of modern chemistry. *Current Science*, 1985. *Journal of Scientific & Industrial Research*, 1976. *Problems in Quantum Chemistry* Poul Jørgensen, Jens Oddershede, 1983. **Reviews in Computational Chemistry, Volume 14** Kenny B. Lipkowitz, Donald B. Boyd, 2009-09-22. THIS VOLUME WHICH IS DESIGNED FOR STAND ALONE USE IN TEACHING AND RESEARCH FOCUSES ON QUANTUM CHEMISTRY AN AREA OF SCIENCE THAT MANY CONSIDER TO BE THE CENTRAL CORE OF COMPUTATIONAL CHEMISTRY. TUTORIALS AND REVIEWS COVER HOW TO OBTAIN SIMPLE CHEMICAL INSIGHT AND CONCEPTS FROM DENSITY FUNCTIONAL THEORY CALCULATIONS. HOW TO MODEL PHOTOCHEMICAL REACTIONS AND EXCITED STATES AND HOW TO COMPUTE ENTHALPIES OF FORMATION OF MOLECULES. A FOURTH CHAPTER TRACES CANADIAN RESEARCH IN THE EVOLUTION OF COMPUTATIONAL CHEMISTRY. ALSO INCLUDED WITH THIS VOLUME IS A SPECIAL TRIBUTE TO QCPE FROM REVIEWS OF THE SERIES. *Reviews in Computational Chemistry* proves itself an invaluable resource to the computational chemist. This series has a place in every computational chemist's library. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* **Journal of the Indian Institute of Science** Indian Institute of Science, Bangalore, 1983. **Chemical Reactivity** Savaş Kaya, Laszlo von

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