Computational Quantum Chemistry

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<u>Computational Quantum Chemistry An Interactive</u> <u>Introduction To Basis Set Theory</u>

Peter W. Atkins, Ronald S. Friedman

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accessible secondary or tertiary literature as a guide for students interested in further reading Sample topics covered in Perspectives on Structure and Mechanism in Organic Chemistry include Fundamental concepts of organic chemistry covering atoms and molecules heats of formation and reaction bonding models and double bonds Density functional theory quantum theory of atoms in molecules Marcus Theory and molecular simulations Asymmetric induction in nucleophilic additions to carbonyl compounds and dynamic effects on reaction pathways Reactive intermediates covering reaction coordinate diagrams radicals carbenes carbocations and carbanions Methods of studying organic reactions including applications of kinetics in studying reaction mechanisms and Arrhenius theory and transition state theory A comprehensive yet accessible reference on the subject Perspectives on Structure and Mechanism in Organic Chemistry is an excellent learning resource for students of organic chemistry medicine and biochemistry. The text is ideal as a primary text for courses entitled Advanced Organic Chemistry at the upper undergraduate and graduate levels **Basis Sets in Computational Chemistry** Eva Perlt, 2021-05-06 This book addresses the construction and application of the major types of basis sets for computational chemistry calculations In addition to a general introduction it includes mathematical basics and a discussion of errors arising from incomplete or inappropriate basis sets The different chapters introduce local orbitals and orbital localization as well as Slater type orbitals and review basis sets for special applications such as those for correlated methods solid state calculations heavy atoms and time dependent adaptable Gaussian bases for quantum dynamics simulations This detailed review of the purpose of basis sets their design applications possible problems and available solutions provides graduate students and beginning researchers with information not easily obtained from the available textbooks and offers valuable supporting material for any quantum chemistry or computational chemistry course at the graduate and or undergraduate level This book is also useful as a guide for researchers who are new to computational chemistry but are willing to extend their research tools by applying such methods **Computational Quantum Chemistry** Charles M. Computational Chemistry Errol G. Lewars, 2007-05-08 Computational chemistry has become extremely Quinn,2002 important in the last decade being widely used in academic and industrial research Yet there have been few books designed to teach the subject to nonspecialists Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike The book provides an overview of the field explains the basic underlying theory at a meaningful level that is not beyond beginners and it gives numerous comparisons of different methods with one another and with experiment The following concepts are illustrated and their possibilities and limitations are given potential energy surfaces simple and extended H ckel methods ab initio AM1 and related semiempirical methods density functional theory DFT Topics are placed in a historical context adding interest to them and removing much of their apparently arbitrary aspect The large number of references to all significant topics mentioned should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers **Subject Guide**

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