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Elementary Quantum Chemistry. As the author notes in the Preface to this valuable text, experimental chemists have moved past studying the average behavior of atoms or molecules "to probe the step-by-step behavior of individual atoms and molecules as they collide, form 'transition states,' and ultimately form products."

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Elementary Quantum Chemistry. Useful introductory course and reference covers origins of quantum theory, Schrödinger wave equation, quantum mechanics of simple systems, electron spin and many-electron systems, the quantum states of atoms, the Hartree-Fock self-consistent field method, the electronic structure of molecules, semiempirical molecular orbital methods, more.

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Elementary Quantum Chemistry, Second Edition. As the author notes in the Preface to this valuable text, experimental chemists have moved past studying the average behavior of atoms or molecules "to probe the step-by-step behavior of individual atoms and molecules as they collide, form 'transition states,' and ultimately form products."

~~Elementary Quantum Chemistry, Second Edition~~

This introductory course — developed by the former chairman of the chemistry department at the University of New Hampshire — covers, among other topics, the origins of the quantum theory, the Schrödinger wave equation, the quantum mechanics of simple systems, the rigid rotator, the hydrogen atom, electron spin and many-electron systems, the quantum states of atoms, the Hartree-Fock self-consistent field method, the electronic structure of molecules, and semi-empirical molecular orbital ...

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A Brief Review of Elementary Quantum Chemistry (PDF 50p) This note covers the following topics: Motivation for Quantum Mechanics, The Schrodinger Equation, Postulates of Quantum Mechanics, Some Analytically Soluble Problems, Approximate Methods, Molecular Quantum Mechanics, Solving the Electronic Eigenvalue Problem. Author(s): C. David Sherrill

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Useful introductory course and reference covers origins of quantum theory, Schrödinger wave equation, quantum mechanics of simple systems, electron spin, quantum states of atoms, Hartree-Fock self-consistent field method, more. 1990 edition.

Useful introductory course covers origins of quantum theory, Schrödinger wave equation, quantum mechanics of simple systems, electron spin, the quantum states of atoms, the Hartree-Fock self-consistent field method, more.

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The Center for Computational Quantum Chemistry (CCQC) at the University of Georgia in Athens, Georgia, offers the full text of the August 1997 paper entitled "A Brief Review of Elementary Quantum Chemistry," written by C. David Sherrill. The paper highlights quantum mechanics, the Schrodinger equation, postulates of quantum mechanics, and molecular quantum mechanics, as well as some analytically soluble problems.

Classic undergraduate text explores wave functions for the hydrogen atom, perturbation theory, the Pauli exclusion principle, and the structure of simple and complex molecules. Numerous tables and figures.

This graduate-level text explains the modern in-depth approaches to the calculation of electronic structure and the properties of molecules. Largely self-contained, it features more than 150 exercises. 1989 edition.

The aim of this book is to give a simple, short, and elementary introduction to the second quantized formalism as applied to a many-electron system. It is intended for those, mainly chemists, who are familiar with traditional quantum chemistry but have not yet become acquainted with second quantization. The treatment is, in part, based on a series of seminars held by the author on the subject. It has been realized that many quantum chemists either interested in theory or in applications, being educated as chemists and not as physicists, have never devoted themselves to taking a course on the second quantized approach. Most available textbooks on this topic are not very easy to follow for those who are not trained in theory, or they are not detailed enough to offer a comprehensive treatment. At the same time there are several papers in quantum chemical literature which take advantage of using second quantization, and it would be worthwhile if those papers were accessible for a wider reading public. For this reason, it is intended in this survey to review the basic formalism of second quantization, and to treat some selected chapters of quantum chemistry in this language. Most derivations will be carried out in a detailed manner, so the reader need not accept gaps to understand the result.

One of the key components of modern physics, quantum mechanics is used in such fields as chemistry, electrical engineering, and computer science. Central to quantum mechanics is Schrödinger's Equation, which explains the behavior of atomic particles and the energy levels of a quantum system. Robert Gilmore's innovative approach to Schrödinger's Equation offers new insight into quantum mechanics at an elementary level. Gilmore presents compact transfer matrix methods for solving quantum problems that can easily be implemented on a personal computer. He shows how to use these methods on a large variety of potentials, both simple and periodic. He shows how to compute bound states, scattering states, and energy bands and describes the relation between bound and scattering states. Chapters on alloys, superlattices, quantum engineering, and solar cells indicate the practical application of the methods discussed. Gilmore's concise and

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elegant treatment will be of interest to students and professors of introductory and intermediate quantum courses, as well as professionals working in electrical engineering and applied mathematics.

Ideas of Quantum Chemistry shows how quantum mechanics is applied to chemistry to give it a theoretical foundation. The structure of the book (a TREE-form) emphasizes the logical relationships between various topics, facts and methods. It shows the reader which parts of the text are needed for understanding specific aspects of the subject matter. Interspersed throughout the text are short biographies of key scientists and their contributions to the development of the field. Ideas of Quantum Chemistry has both textbook and reference work aspects. Like a textbook, the material is organized into digestible sections with each chapter following the same structure. It answers frequently asked questions and highlights the most important conclusions and the essential mathematical formulae in the text. In its reference aspects, it has a broader range than traditional quantum chemistry books and reviews virtually all of the pertinent literature. It is useful both for beginners as well as specialists in advanced topics of quantum chemistry. The book is supplemented by an appendix on the Internet. * Presents the widest range of quantum chemical problems covered in one book * Unique structure allows material to be tailored to the specific needs of the reader * Informal language facilitates the understanding of difficult topics

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