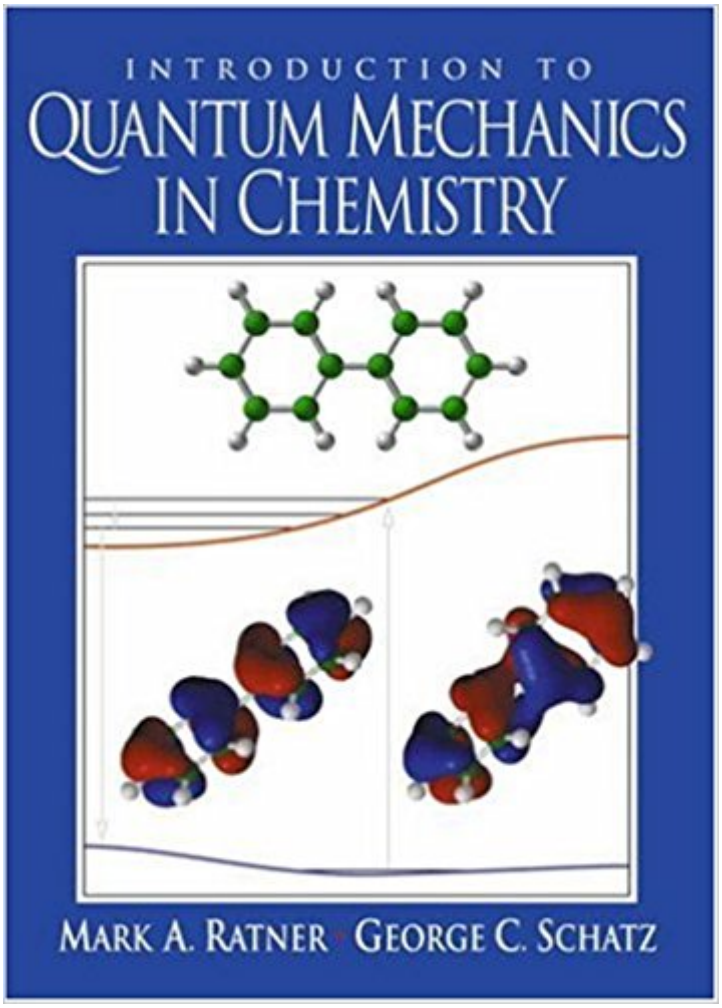
Introduction To Quantum Mechanics In Chemistry



Synopsis

This book serves as a self-study guide to familiarize users with the crucial language of modern chemistry science. It provides a background of electronic structure programs, and includes worked examples in problem solving and computer exercises. For computational chemists, materials scientists, and chemical engineers who want to learn more about their field without unnecessary complexity, detail, or formalism.

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Preface Quantum mechanics, particularly quantum chemistry, is a crucial part of the language of modern chemical science. Terms such as pÃ•â ¬-dÃ•â ¬ interaction, symmetry-forbidden reactions, bond-order/bond-energy relationships, hypervalency, and exchange repulsion are typical of those that arise in contemporary discussions of chemical structure and properties. This language is a powerful one with which the contemporary chemical scientist needs to be familiar. The language starts with quantum mechanics, and that brings with it some formal and mathematical impediments.

Most chemists do not intend to be theorists or even traditional physical chemists. For them, many of the niceties and formal elegances of quantum mechanics are really irrelevant, since their aim is a more utilitarian one: to use quantum chemistry to understand the molecular problems or the materials problems that arise in their own research and understanding. Within the past 15 years, the broad applicability and availability of appropriate modeling tools has made quantum chemical techniques part of the arsenal of most chemists. Indeed, more electronic structure calculations are published by people who do not call themselves physical chemists than by people who do! Given this situation, we felt that it was appropriate to write a text focused on the language of quantum chemistry and the tools that it makes available. The approach is straightforward: It attempts to avoid all unnecessary complexity, detail, and formalism. The book is not written for theorists; rather, it is intended to allow all chemical scientists to become familiar with the language of quantum chemistry and with the use of many of its most important tools. The book is designed to provide an integrated approach to the conceptual development of quantum chemistry and to its application in current research questions. It is intended to be modest and straightforward, easily completed in its entirety either in a one-semester formal course (at the advanced undergraduate or beginning graduate level) or as a self-study document that can be completed in about 50 hours of reading, problem solving, and computer exercises. The in-chapter exercises are intended to demonstrate problem-solving methods. We recommend trying to solve them before looking at the solution that is given. (Answers, to odd-numbered exercises are provided in the appendix to this text. Full solutions are available to instructors by contacting Prentice Hall and requesting ISBN 0-13-015487-3.) The problems at the end of each chapter are of differing levels of difficulty; some (for example, Problems 2.12, 6.5, 8.8, 8.11,13.4, 14.11, and 15.6) contain important thematic material. The computer exercises (especially those in Chapter 14) are an important part of the book, just as, to most chemists, computational applications are arguably the most important contribution of quantum chemistry. The methods discussed in Chapters 11,12, and 14 are available through the use of a large number of commercial and freeware codes. Such software permits the chemist to answer, more accurately and efficiently, many of the questions involving molecular structure and response that arise in understanding the behavior of molecules. The book is intended for chemists, materials scientists, and chemical engineers who wish to learn the language of quantum chemistry and the computational methods that it provides. The volume can also serve as a bare-bones introduction for those who intend to pursue quantum chemistry more deeply, perhaps supplemented by some of the texts that are discussed in the bibliographies at the end of each chapter. Our more advanced book, Quantum Mechanics in Chemistry (Englewood Cliffs, NJ-Prentice Hall, 1993), is organized so that

one can jump directly from Chapter 14 of the present book to Chapter 3 of that one, so as to provide enough material for an entire year's course on quantum chemistry. It is our aim in this text to provide an introduction to quantum chemistry that can be used with ease (and, we hope, with some pleasure) by most chemists. We are grateful to Margaret and to Nancy for allowing us to spend even more time than usual in the completion of this book, and to John Challice and his colleagues at Prentice Hall for inspiration in writing and help in assembling the book. We also thank Fred Northrup for the spectra in Chapter 15; Janet Goranson, who suffered through several nearly fatal wordprocessor upgrades, for her expert typing; our students, who suffered through several early versions -of the book, for their useful and challenging suggestions. We thank Brian Hoffman, Northwestern Unversity; John Head, University of Hawaii; W Vern Hicks, Jr., Northern Kentucky University; and Duane Swank, Pacific Lutheran University, for their careful review of the manuscript for this book. Mark A. Ratner ratner@mercury.chem.nwu.edu George C. Schatz schatz@chem.nwu.edu

From a beginners point of view, it was not helpful. I bought this book because it was a prerequisite for my class. The descriptions and explainations were brief. It did not show their work when working equations. All around I did not like the book. Maybe if you're familiar with the subject it may be of some use to you and their explainations of the subject matter may be acceptable, but since this was my first time being introduced to the subject coupled with my professors expectations of being able to work problems, it did not do much for me. I switched to another text that I found very helpful.Quantum Chemistry. That book with its solution manual was ideal for my situation.

I made an effort to use this text for undergraduate pchem... our professor was trying it out (Berkeley.) I abandoned the book for lack of explanation and depth, it more read as a book of equations, but sometimes the derivations were not even clear.I wish I could go into further detail; alas I sold it (for way less, the binding was horrific and began to fall apart within mere weeks!) Suffice it to say, IMO you should save your money!fwiw, I recommend the Atkins & Friedman text Molecular Quantum Mechanics along with Griffith's Quantum Mechanics. Much more helpful books that allowed me to get an above average grade in the class.hth

buy it if it's required for class, but it is difficult to find what you're looking for, and not so easy/fun to read. It serves, but maybe not as well as some other book could.

The book looked like it had been sat on by elephants and the spine was not attached to the pages. I wanted to send it back, but I needed it for homework. Overall this was a bad buy, I hope whoever sold this to me would have taken better care of it.

I thought this book read and functioned somewhat like a magazine on Quantum Mechanics. Often the gritty details and sometimes even the elegant parts were glossed over, or entirely left out. The book was easy to read on a surface level, but sometimes difficult to extract meaningful knowledge form. I found myself working through a variety of other textbooks to help me understand what Ratner and Schatz left out.On the other hand the problems from the text are very good, they are difficult but illustrative of some of the finer points of concepts.All in all its a nice book to have around but it is most certainly not my go-to choice for QM.

I don’t know why more people don’t use this book or the authors’ more advanced version, "Quantum Mechanics in Chemistry", but I think they are both fantastic. This book in particular is very clearly written with explicit examples and and relevant end-of-chapter exercises...with detailed solutions to the odds (very rare)! It focuses more on on many-electron problems and methods, which is essential for understanding chemical problems. If your an undrgraduate chemistry major or a beginning graduate student in chemistry who needs a refresher before taking a more advanced class, you would be well served by this book.

Quantum Gravity: An Elementary Introduction to Quantum Gravity and Spinfoam Theory (Cambridge Monographs on Mathematical Physics) Study Guide: Ace Organic Chemistry I - The EASY Guide to Ace Organic Chemistry I: (Organic Chemistry Study Guide, Organic Chemistry Review, Concepts, Reaction Mechanisms and Summaries) Ace General Chemistry I and II (The EASY Guide to Ace General Chemistry I and II): General Chemistry Study Guide, General Chemistry Review Introduction to Quantum Mechanics Quantum Chemistry & Spectroscopy Plus MasteringChemistry with eText -- Access Card Package (3rd Edition) (Engel Physical Chemistry Series) Recent Advances in the Theory of Chemical and Physical Systems: Proceedings of the 9th European Workshop on Quantum Systems in Chemistry and Physics ... in Theoretical Chemistry and Physics)