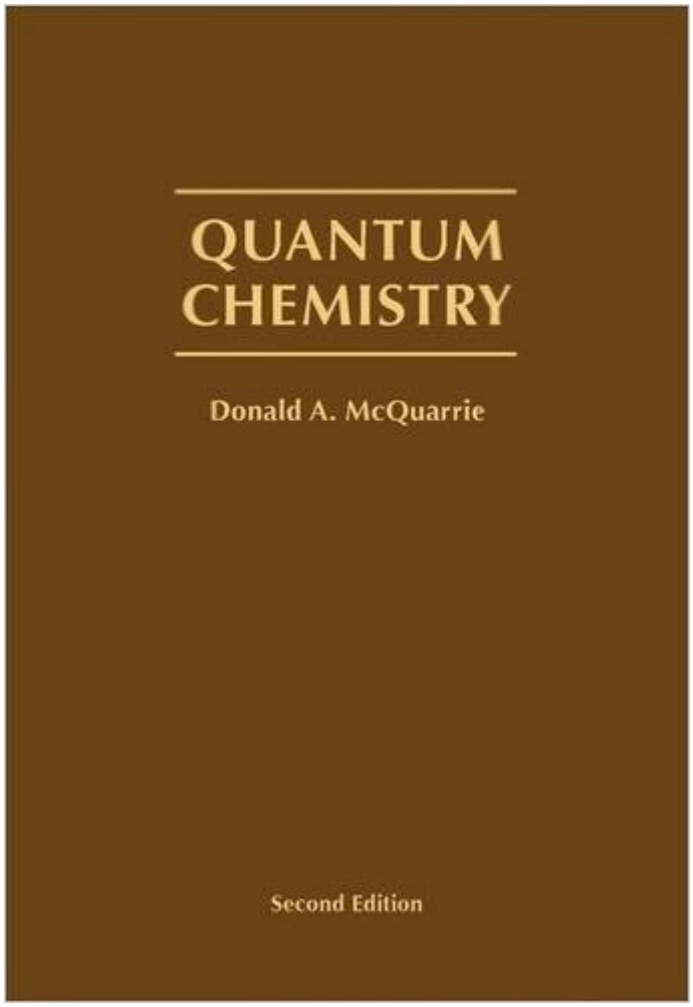
Quantum Chemistry



Synopsis

After twenty-four years in print, Don McQuarrie has now updated his landmark "Quantum Chemistry". Perhaps the biggest change in the years since the first edition is the proliferation of computational chemistry programs that calculate molecular properties. McQuarrie has presented step-by-step SCF calculations of a helium atom in Chapter 9 and a hydrogen molecule in Chapter 10, in addition to including an entire chapter on the Hartree-Fock method and post-Hartree-Fock methods for the calculation of molecular properties. The book also uses problems to encourage the use of an invaluable National Institute of Science and Technology (NIST) website that lists experimental data and the results of various ab initio calculations for hundreds of molecules.

Book Information

Hardcover: 690 pages

Publisher: University Science Books; 2 edition (August 15, 2007)

Language: English

ISBN-10: 1891389505

ISBN-13: 978-1891389504

Product Dimensions: 6.9 x 1.4 x 10.3 inches

Shipping Weight: 3 pounds (View shipping rates and policies)

Average Customer Review: 4.6 out of 5 starsÂ Â See all reviewsÂ (26 customer reviews)

Best Sellers Rank: #87,414 in Books (See Top 100 in Books) #2 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #19 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Physical Chemistry #331 inÂ Books > Textbooks > Science & Mathematics > Chemistry

Customer Reviews

after a semester of suffering through atkins physical chemistry 9th edition for thermodynamics, I really like the fact that my instructor decided to use quantum chemistry written by mcquarrie for the quantum part of pchem. Mcquarrie definitely is a better writer than atkins, whose writing/explanations leaves students more confused with his habit of pulling equations out of thin air with no explanation and "it is what it is" attitude.McQuarrie’s book states that it was written in such a way that you should do alright with just a basic level of calculus. While that might be true, I think you’d have to be pretty good at math in general to do well in pchem. For an intro quantum book, I think mcquarrie’s is the best option out there and it’s no wonder it’s been around for 20+ years.The book was also written with latex so the writing is very neat. The book cover is also very conservative

and professional looking, resembling that of a reference book that you might keep on your shelf one day.Only con, the binding of this book SUCKS...

I used this book as a supplement to Levine in an honors Pchem class. All in all, I was pleasantly surprised by the readability of McQuarrie's text. The material is clearly presented, the progression is very well structured. McQuarrie's lightweight presentation and mathematical asides made my journey through the material relatively smooth and rapid; a refreshing breeze after the heavy roaring of Levine's more exacting and thorough treatment of the subject.As a bonus for those of us who like to learn by doing, a very well written and comprehensive solution manual is available for the text.

I've always thought that if you master a subject should be able to explain easily. That is the case with this book. The author not only dominates the issues, but in this edition features chapters of math, beautifully described, to help understand the rest of the book. Whether you work with semiconductors, solar cells, conductive polymers, nanoscience or, in general, want to learn solid state physics, this book is essential in your library. I use it as a textbook in a graduate course entitled: Functional properties of crystals. This course is taken from physical to chemical engineers and geologists, and the book is helpful regardless of specialty.

This book is a well written introduction to quantum chemistry. I recommend it highly for undergrads taking their first quantum course. It probably could be used to help with a Modern Physics course as well. As a chem major it worked well for me during my first exposure to quantum. Actually enjoyable and worthwhile to read even if it does not have as much depth as it could.

This was my quantum chemistry textbook at the university and IÃ¢Â Â™ve recently returned to it for review. It is a remarkably straightforward presentation of quantum mechanics and quantum chemistry. It is rigorous and thorough but very well organized and easy to follow. Terms are explained clearly and the examples demonstrate the application of the basic principles very well. One reason I am impressed with this text is because of the disorganized and impenetrable presentation of identical material I have seen in other texts. Quantum mechanics is not simple but it need not be inaccessible. Once you have a basic understanding of the vocabulary and mathematical tools involved itÃ¢Â Â™s actually not that difficult. But you need a good presentation, which is what this text provides.

ORIGINAL REVIEW: Overall, this is a great text for an undergraduate chemist’s introduction to quantum mechanics. The writing and derivations are clear, figures are thoughtfully used, the progression of the chapters is logical, and the index is relatively comprehensive; this makes for a very readable and useful book to both learn from and use as a quick reference. The end-of-chapter problems are also fantastic. There are tons of them, and they span the spectrum from short and easy variations of in-chapter examples to full-fledged proofs. In the more difficult problems and proofs the author walks the student through the process as a good tutor would nudge a student in the right direction.Compared to a physics text, it spends much more time on atomic/molecular applications of quantum mechanics. Rotational and vibrational spectroscopies are covered at a basic level, and chemical bonding is covered in relative detail. On the flip side, some other really interesting applications are left out.Some things I didnÃ¢Â Â™t care for:-Some important concepts are left to the problems. Tunneling, for example, was introduced in a long-form problem that went something like this: "The idea of quantum mechanical tunneling can be demonstrated by a wave incident on a potential energy step (shows a picture). Tunneling is important in a variety of chemical processes. (gives the equations you need, tells what they mean). Now solve for blah blah blah." The question then asked what those things we just found might mean. I don’t think it’s a good idea to introduce an idea as important as tunneling in a problem, as well thought-out as that problem may be.- McQuarrie typically uses the very simplest case to derive and/or explain topics, and this caused a few spots of frustration for me, especially in the later sections.- Spin gets a very basic treatment; my recollection is that it got perhaps two pages, just enough so that McQuarrie could talk about wave function symmetry and Slater determinants.- ThereÃ¢Â Â™s not much talk about Ã¢Â Âœwhat it all meansÃ¢Â Â• - the book generally treats the subject as a useful tool rather than a subject thatÃ¢Â Â™s interesting on its own.UPDATE: My original review was a 5-star, but I docked one. This book is perfect for an intro course aimed at teaching the basic ideas of quantum mechanics and its applications to chemistry. For most chemists, thatÃ¢Â Â™s totally sufficient. For those who want to/need to study more quantum mechanics, the book is a little shallow. The relationship between wave functions and vectors, and what the Ã¢Â Âœstate Ã¢Â Â• of a system really means, werenÃ¢Â Â™t really emphasized. Similarly, I wish that what matrices and linear algebra have to do with the subject came across more clearly. These are all mentioned, but treated more as asides. These concepts are super important to understand if one wants to go further with the subject, but I also think they are essential to a basic treatment as well. Still a good book though. I used it in a class taught by a great professor, and by the end of the semester I really loved the subject.

I needed this book for a class i a taking but it is definitely not the best book to learn quantum chemistry from. It constantly skips important math steps in all of the example problems, so if you don’t have fresh knowledge of calculus or multivariable calculus this is not the book for you. On the bright side each chapter ends with a math chapter is needed to understand other parts of the book so you’re not left completely in the dark.

Quantum Mechanics! The How’s and Why’s of Atoms and Molecules - Chemistry for Kids - Children’s Chemistry Books Surviving Chemistry Workbook: High School Chemistry: 2015 Revision - with NYS Chemistry Reference Tables The Quantum World: Quantum Physics for Everyone Multiconfigurational Quantum Chemistry Atoms in Molecules: A Quantum Theory (International Series of Monographs on Chemistry) Introduction to Quantum Mechanics: in Chemistry, Materials Science, and Biology (Complementary Science) Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Quantum Chemistry Quantum Chemistry and Spectroscopy (3rd Edition) Sterling Test Prep CLEP Chemistry Practice Questions: High Yield CLEP Chemistry Questions Sterling DAT General Chemistry Practice Questions: High Yield DAT General Chemistry Questions MCAT Chemistry and Organic Chemistry: Content Review for the Revised MCAT Principles of Colloid and Surface Chemistry, Third Edition, Revised and Expanded (Undergraduate Chemistry: A Series of Textbooks) Physical Chemistry Plus MasteringChemistry with eText -- Access Card Package (3rd Edition) (Engel Physical Chemistry Series) Clinical Chemistry: Techniques, Principles, Correlations (Bishop, Clinical Chemistry) Chemistry: An Introduction to General, Organic, and Biological Chemistry (12th Edition) Glencoe Physical iScience Modules: Chemistry, Grade 8, Student Edition (GLEN SCI: CHEMISTRY) Kendall / Hunt Chemistry: Discovering Chemistry You Need To Know Quantum Physics for Babies (Volume 1) Quantum Information for Babies (Physics for Babies) (Volume 5)