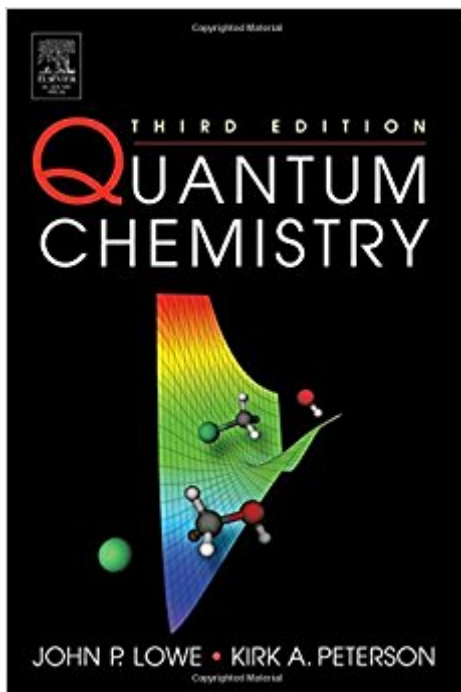


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# Quantum Chemistry, Third Edition



## Synopsis

Lowe's new edition assumes little mathematical or physical sophistication and emphasizes an understanding of the techniques and results of quantum chemistry. It can serve as a primary text in quantum chemistry courses, and enables students and researchers to comprehend the current literature. This third edition has been thoroughly updated and includes numerous new exercises to facilitate self-study and solutions to selected exercises. Assumes little initial mathematical or physical sophistication, developing insights and abilities in the context of actual problems. Provides thorough treatment of the simple systems basic to this subject. Emphasizes UNDERSTANDING of the techniques and results of modern quantum chemistry. Treats MO theory from simple Huckel through ab initio methods in current use. Develops perturbation theory through the topics of orbital interaction as well as spectroscopic selection rules. Presents group theory in a context of MO applications. Includes qualitative MO theory of molecular structure, Walsh rules, Woodward-Hoffmann rules, frontier orbitals, and organic reactions. Develops MO theory of periodic systems, with applications to organic polymers.

## Book Information

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## Customer Reviews

"This new edition is based closely on the already outstanding second edition, with the addition of a co-author and appropriate updating, reworking, and elaboration of the material. The overall quality of this book is on par with the excellent work by Ira N. Levine, Quantum Chemistry (5th ed., 2000). The authors aim at conceptual understanding as well as mathematical development. The book

includes a large and varied set of homework problems, together with hints and brief solutions. A distinctive feature is the inclusion of some multiple-choice questions. Generous numbers of more traditional problems are provided as well." Summing Up: Highly recommended. Upper-division undergraduates through professionals. A. Viste, emeritus, Augustana College, CHOICE, September 2006, Vol. 44, No. 1 "The book is very well written and in contrast to many other texts it focuses on the understanding of the concepts. This should provide the reader the knowledge to evaluate the various computation methods, and to make informed choices about specific quantum chemical methods for a given problem. Another attractive feature of this book are the end of chapter problems. In summary, this is an excellent text for a graduate level introduction to quantum chemistry and every teacher of these types of classes should give this text serious consideration." S. Saebo, Mississippi State University, Starkville, MS, USA, STRUCT CHEM (2006)

The updated classic now includes worked-out examples in each chapter!

Full of annoying, confusing mistakes. It was also oversimplified in explaining the concepts. There are many better books on quantum out there.

Well-written, and easier to understand than a lot of quantum/physical chemistry books. I have liked it thus far!

really good and like a new book. Seems that haven't ever been used.

If you are looking for an introductory text for Quantum Chemistry, well, here it is. Lowe understands something very important about writing introductory texts, something that most authors don't grasp. That being that an introductory text isn't simply a book that talks about the foundations of the given subject, but also speaks to someone who is inexperienced in the subject. Lowe has this down to almost an art; most subjects are sufficiently explained with little fluff or unnecessary technical jargon. The book isn't quite as expansive as say, McQuarrie's Physical Chemistry, but what is? The essentials are explained with the necessary depth and any mathematics involved are explained in the Appendices. The book stumbles when Lowe tries to explain more qualitative ideas, like LCAO. Without the structure of mathematics, the book seems to falter quite a bit. After several readings, I still had no idea what Lowe was talking about in the latter sections of chapter 7. Nevertheless, this is a pretty strong text.

I am perhaps marginally biased towards Lowe's book, I used it as an undergraduate taking graduate quantum chem with a very fine lecturer. Lowe's book is intended for a general introduction to quantum chemistry & molecular orbital theory - this is a book that will be kept and used even by those chemists who are not physical and/or theoretical chemists. He emphasizes the basics and physical understanding over developing the material in a more pure mathematical fashion. As for the list of errors that the previous reviewer mentioned, I can only wonder if those same errors were the ones corrected on the errata sheet that was handed out to me in class. As I'm finally in graduate school taking quantum again, we're using Levine's text as well as Fayer's text. I think Lowe has prepared me beautifully by having instilled the big picture in my head. If you're really serious about your Q.M., you'd supplement with a physics text anyway (Shankar, Merzbacher, Liboff, etc). But that's more for clearing up the physics details than anything else, IMHO.

I used this book for guided independent study in my senior year as a Chemical Engineering undergraduate. To learn from this book is easy. Lowe does a great job integrating the mathematics into his work. Some authors tend to get bogged down in math, and others (in my mind incorrectly) insist that you don't need to understand the math to understand quantum chemistry. Lowe strikes the right balance and shows what the mathematics mean, chemically. Additionally, the exercises are well written and useful. Including solutions to some of the exercises is a must for a book of this level, and I'm glad to see it done here. Two complaints: Some color diagrams would make for easier visualization of some of the more difficult topics...and more efforts at introducing computer software commonly used in quantum chemistry (eg. Gaussian) would have been nice. All in all, a good book, much better than most quantum chemistry texts available.

I'm currently finishing up a self-directed course on quantum chemistry. My two principle sources are Lowe's book and Levine's book, and I find that the combination works fairly well. Unlike Levine, Lowe is not a precise writer and often skips details. I have also found mathematical and conceptual mistakes in some parts. You might not notice them in a quick read through but under close scrutiny they present a problem. He's definitely more a chemist than a physicist... The end result is that if I try to read his book first, I inevitably become confused. However, where he shines is in bringing together the big picture in words \*once you've already understood the details\*. Thus my typical strategy is to read Levine to get a wonderfully detailed and accurate lesson, and then read the same topic in Lowe to bring it all together. If I had to buy only one, Levine is definitely the way to go.

Assumes little mathematical sophistication. Excellent book for the beginning student of quantum chemistry. Suitable for junior/senior undergraduate or beginning graduate students. Contains a wealth of practice exercises with detailed answers to most. The latter part of the book is concerned with practical applications of quantum chemistry with an excellent and readable introduction to modern computational methods. Helps students get a practical and qualitative feel for quantum chemistry and provides an excellent foundation on which to base later study. Covers quantum basics, group theory, Hartree-Fock-based approximations, MO/AO theory and applications to periodic systems to name but a few of the well-chosen topics.

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