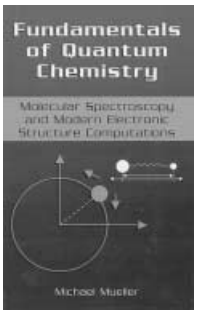
Fundamentals of Quantum Chemistry. By *Michael Mueller.* Kluwer Academic/Plenum Publishers, New York 2001. 265 pp., hardback $ 69.50.—ISBN 0-306-46596-5



Electronic-structure calculations have long become a standard tool also for experimentalists in chemistry and related disciplines, thanks to the numerous commercially available quantum-chemistry software packages. The large degree of standardization of many computational methods—such as the use of well-defined basis sets, such as, 6-31G, 6-31G*, etc.—has enabled the nonexpert to use these methods according to the 'back box' principle. This, of course, can be dangerous if the user does not have a sound knowledge of the advantages and limitations of the individual methods. Teaching the necessary theoretical background as well as gathering first 'hands-on' experiences, therefore, form an important part of any chemistry degree course, today.

In this context, the present textbook is aimed mainly at first and second year undergraduate students with only minimal mathematical and chemical knowledge.

According to the author, the book should offer them an introduction to quantum chemistry as close as possible to practical application. As indicated by the book's subtitle 'Molecular Spectroscopy and Modern Electronic Structure Computations', another focus, apart from electronic structure calculations, is on interpretation and prediction of vibrational and rotational spectra using quantum mechanics.

In the first chapter, the Newtonian and Hamiltonian equations of motion of classical mechanics are introduced extremely briefly and applied to the harmonic oscillator.

Chapter 2 introduces the fundamental concepts of quantum mechanics and goes back to the usual 1-d and 3-d particle-in-a-box model, which is extended in Chapter 3 to the particle-on-a-ring and the particle-on-a-sphere.

Besides the numerous example calculations, the many boxes labeled 'Chemical Connection' and 'Point of Further Understanding', which point the student to chemical applications of the abstract fundamental theory and stimulate deeper thought or discussion, respectively, add particular value to this book. Thus, the author early establishes, for example, the connection between the harmonic oscillator and vibrational spectroscopy.

A central role is played by Chapter 4, in which the variational principle as well as perturbation theory are treated. Both of these approximation techniques are used several times throughout the further course of the book.

Chapter 5 deals with the quantum-mechanical harmonic oscillator, preparing the reader for the following two chapters on vibrational and rotational spectroscopy of diatomic and polyatomic molecules. It appears as if Michael Mueller has expressed his competence here in particular as he discusses a number of different orders of approximation and repeatedly refers to the interplay of theory and experiment.

Finally, the last two chapters are dedicated to the electronic structure of atoms (Chapter 8) and molecules (Chapter 9). First, the solutions of the Schrödinger equation for the one-electron atom are deduced, which then serve as a starting point for solving the helium atom by employing the approximation techniques of Chapter 4. In the section on many-electron atoms the concept of Hartree-Fock calculations is explained qualitatively for the first time subsequent to Slater's rules.

The LCAO approximation is presented briefly within the treatment of the hydrogen molecule cation, before addressing elementary fundamentals of molecular mechanics. Thereupon Hartree-Fock theory is dealt with in more depth and the problems associated with basis sets noted. Correlated methods, except for a short trip into Møller – Plesset perturbation theory, are only vaguely hinted at. A short listing of semiempirical methods is followed by a rather superficial introduction to density functional theory.

The numerous tables in the last chapter illustrating the accuracy of bond lengths and dissociation energies calculated with various electronic-structure methods are very helpful. Apart from that, this is, in my opinion, the weakest chapter of the entire book, not least because a substantially more detailed treatment may be expected from both the title and the subtitle of this textbook. Moreover, a number of factually incorrect formulations can be found in the text—particularly in the section on density functional theory.

In conclusion, the current textbook is generally well suited as a basis for an introductory course of lectures on quantum mechanics for chemistry undergraduates. A positive aspect is the motivating frequent pointing out of the relationship between fundamental theory and practical chemical applications. I consider that, in this context, the chapter on vibrational and rotational spectroscopy is the most successful. The problems at the end of each chapter are superbly suited for supplementary tutorials.

Unfortunately, references for further reading are missing completely, with the exception of Chapter 6. Furthermore, the often shameful quality of many viewgraphs (some curves seem to be drawn by hand!) as well as the large number of errors, which can not always be attributed to printing or typographical errors, have to be critizised. Striking is, for example, the repeated use of the word 'affect' instead of the expected 'effect'. The most serious criticism is that this book, contrary to the author's declared goal, does not enable the reader to use competently a quantum chemistry software package. In this category there are by far better textbooks, such as, for example, Frank Jensen's 'Introduction to Computational Chemistry'.

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