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Book Reviews

J. Goodisman: Contemporary Quantum Chemistry. New York: Plenum Press 1977. 376 pp., price: US-$39.00

Behind this ambitious title we find an introductory text on quantum chemistry conceived for chemistry seniors with no further exposure to theoretical chemistry. The contents are rather conventional and by no means exhaustive. Eleven chapters cover the application of the time-independent Schrödinger equation to atomic and molecular structure, two further chapters introduce symmetry and time-dependence. As usual particle in a box, harmonic oscillator, hydrogen to lithium atoms, hydrogen molecule, diatomic and a few standard polyatomic molecules are treated. From the methods variation principle, independent particle model, screening, valence bond and MO method are included. Different from other books is the way of presentation. The author feels, and rightfully so, that the chemistry student in general is poorly prepared in mathematics and physics for an immediate grasp of quantum chemistry. So he simplifies as far as possible and is very explicit on derivations. Typical section titles are "What One Can Do with Wave Functions" or "A Dose of Mathematics". The latter section, for instance, expresses in understandable language what an operator is and proceeds to linear and Hermitian operators. Most sections of this type are very well done and show unusual originality in an introductory text. However, there is danger in carrying simplifications too far and this book is not free of it. For instance, very early on page 5 the author describes the nature of an electron this way: "It is as if the electron, rather than being a particle located at some point at each instant of time, is pulverized or spread out like a cloud of dust and spread over a relatively large volume of space". The discriminating "as if" gets lost and the pulverized picture of the electron is adopted in many following figures. Furthermore the clouds rotate and two rotating clouds explain overlap. Thus by initially avoiding the concept of probability the author creates the impression of motion in stationary states. It is helpful that he correctly states somewhere early that particle or wave character appear dependent on the nature of experiment. But it is disturbing that the uncertainty principle is introduced only as a sideline. On the other hand the mathematical simplification is sometimes overdone: pages 22–28 serve on solving differential equations numerically on a level comparable to counting the area of rectangles to solve integrals. This is not only practically useless, but also might create an uneasiness about differential equations. The saved space could have been used to better explain bonding and antibonding on page 252 or justify the neglect of overlap in Hückel methods on page 264. No attempt is made on page 246 to generalize the expectation value of H in a many-electron system. Mistakes or misprints are few: the direction of the force T should be opposite on page 16 and in Fig. 11.10 the ethylene molecule should not be labelled ethane. It is probably in the philosophy of the author that no literature list is given except for a few footnotes. The problems are simple, but instructive.

The overall impression of this book is positive. It stands out against comparable textbooks. Chemistry students with no further plans for theoretical or physical chemistry will appreciate its readability and it might even get some interested in the subject. But who will afford the high price of $39?

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Brian L. Silver (Ed.): Irreducible Tensor Methods. An Introduction for Chemists. New York–San Francisco–London: Academic Press 1976. 226 pp., price: US-$ 26.50 (£18.80)

This book gives an introduction to the theory of irreducible tensor operators and their application in chemical physics. According to the preface, the text is intended for graduated chemists; however, considering chemical education in this country, the book will only be readable for a smaller number of chemists, i.e. those having an exceptionally good knowledge of mathematics and quantum mechanics. From the topical point of view, the book is competitive to the textbooks by Fano and Racah (1959), Griffith (1962), and Judd (1963) and there is quite naturally a rather large overlap with the contents of these books. Nevertheless, there are novel developments in this field treated by Silver, and this makes the new book useful. The subject matter treated in the first three chapters on the algebra of angular momenta, of chapter 6 on the Wigner-Eckart-Theorem, and of chapters 7 and 8 on the 6-j and 9-j symbols will of course also be found in the well-known books by Rose (1957), Edmonds (1968) and by Brink and Satchler (1968).

It is gratifying that a number of obscurities to be found in the above mentioned books, as e.g. the use of the active or passive interpretations of rotations, have been cleared up by the present author.

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