Theoret. chim. Acta (Berl.) 17, 248 (1970)

Recensio

Frank L. Pilar: Elementary Quantum Chemistry. New York-London: McGraw-Hill 1968. 726 pages.

Frank Pilar's book is the first of a number of recent texts on quantum chemistry in general, indicating a need for a new, fresh approach to this subject. The size is impressive for an elementary level text. Is this book going to replace Kauzmann's book in teaching beginning graduate students? The reviewer had the opportunity to test its value during a one-year quantum chemistry course.

There are many features which make it attractive for teaching. Dirac's bra-ket notation is used parallel to the common integral notation. Throughout the book, there are many references to classical and recent pertinent papers which are properly integrated. There is a rigorous mathematical foundation whenever necessary. Many paragraphs are dedicated to explanations of the physical background and refer also to classical analogues, e.g. Lagrangian and Hamiltonian formalisms. Topics include the history of quantum theory, mathematical tools like operators, matrices and group theory, quantum mechanics of simple systems, angular and spin momenta, atomic and molecular structure of diatomics and polyatomics, special techniques like the Hartree-Fock method and a chapter on radiative processes. A strength of the book is that it discusses one topic thoroughly from various aspects; for example, the helium atom is treated in the independent-particle model, then with electronic repulsion, followed by an application of the virial theorem and scaling, finally in the Hartree method, later again in connection with variation, perturbation and Hartree-Fock methods. This gives the student the opportunity to compare the usefulness of various approaches and systematically stresses important facts. There are many tables and figures to make the theory more suggestive. It is not a disadvantage that many of those plus explanations are borrowed from successful predecessors like Eyring, Coulson or Kauzmann. There is a strong influence felt due to Löwdin when the topic of projection operators is brought up. Indeed, never have projection operators been presented in such a useful fashion in an elementary textbook.

However, the attempt of the author to cover a great many details of present quantum chemistry of molecular structure and bonding is probably not what we want in an elementary text. For example, the topic of density matrices cannot be covered adequately in ten pages. On the other hand, students try to exhaust the potential of the text without being satisfied. One wonders whether this topic could not be dropped. The important chapter on group theory is also insufficient, although it was worth trying. The author does not classify groups, nor does he explain what symmetry operations σ_v, σ_h, etc. mean, but uses their properties. On pages 392 he confuses the important explanation of transformations by mixing up unitary and similarity transformations, which were previously correctly defined. A major deficiency is also the placement of radiative processes as Chapter 5, which naturally belongs after an introduction of perturbation theory presented in Chapter 10. In Chapter 12, there is a paragraph on multiplet levels in atoms (pp. 307–309) which does not help the student to clearly figure out which multiplet states are allowed from single-electron l and m values. A minor point is the question why the author uses Δ instead of the now generally adopted S as the notation for the overlap integral. This is a bit unfortunate because a connection with the Kronecker δ is suggestive and the meaning of Pilar's Δ is different from Löwdin's. The length of the text makes it impossible for the reviewer to remark on further details. One final example might characterize the situation in some way. On page 462, there is the well-known correlation chart for homonuclear diatomics. Although a lot of useful remarks are given, there is no simple explanation at this point on how to make use of this chart. It cannot be clear to the student what happens if we bring two carbon atoms together and finally end up with magnesium which has no 3*p*-electrons. And it does not help him either that the Aufbau principle is discussed forty pages later.

The number of errors and misprints is not large for a book of this size. The problem sets are related to the material covered in the text. They are easy and instructive. The index register is appropriate.

The text is so far the best available for teaching. However, in a possible revision the author might guard himself a bit against collecting too much material where clarity and precision is needed. In this sense, the book by Frank Pilar can be recommended and it will be a useful addition to quantum chemistry texts for years to come.

Received March 12, 1970

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