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Book review

H. Primas and U. Müller-Herold: Elementare Quantenchemie. Teubner, Stuttgart 1984

This is a very carefully and intelligently written book. The subject matter is very much the same as in standard introductory textbooks on quantum chemistry, but the presentation is rather unconventional and the main emphasis is on aspects of the theory that are usually not given special attention. In the introduction to quantum mechanics the abstract theory of measurement and the algebra of observables (especially classical observables and superselection rules) play the central role. There is also a nice and sophisticated section on the Galilei kinematics, though the role of spin within this kinematics remains obscure. On the other hand Hilbert space theory or distributions are introduced in the naive, non-rigorous way and the treatment of the variation principle is rather sketchy. Although the authors mention that it is easier to apply quantum mechanics than to understand it, they care more for understanding (whatever this means) and they have some scorn for colleagues who are only concerned with applications.

In the chapter on molecules the Born–Oppenheimer separation of electronic and nuclear motion gets crucial importance, not as an approximation for the calculation of wave functions, but as a singular limit of the theory which implies new classical observables and which is responsible for the very concept of "molecular structure". Rotation and vibration as part of hierarchical structure of molecular systems are treated before the theory of the electronic structure of molecules. The Hartree method is introduced unconventionally as a mean-field theory.

Localized orbitals are seen in context with the best Hartree approximation to Hartree–Fock and this explains why the authors prefer in a very pronounced way the localization criterion of Edmiston and Ruedenberg to that of Boys (although in practice the two criteria mostly lead to indistinguishable results). The H_2 molecule is presented as a case study of successful search for agreement between theory and experiment with increasing accuracy of both experimental and theory.

In the subsequent discussion of standard numerical methods of *ab initio* and semiempirical quantum chemistry it becomes obvious that the authors are only marginally concerned with numerical theory.

The wrong asymptotic behaviour of Hartree–Fock theory for large inter-nuclear distance or the distinction between dynamic and non-dynamic correlation effects are not even mentioned. In order to learn numerical quantum chemistry this is certainly not the text to choose.

While the authors are so much concerned with "understanding" quantum mechanics they care very little for "understanding" the chemical bond (they simply claim that there is no satisfactory valence theory available). They criticize that existing theories can only deal with single molecules, not with classes of compounds (say ketons).

Many nice ideas are found in the epilogue, especially in the section "to the young generation" which contains a massive criticism of the present tendency to teach youngsters orbitals rather than chemical facts.

The term "elementary" in the title can have two extreme meanings (a) "introductory", (b) "fundamental". It seems to me that the weight is more towards (b) and that an initiated reader will take more advantage of this book than a beginner. I do not see a comparable text in English, and I

recommend to non German speaking readers to fresh up their German in order to study this book or at least part of it. Even if one does not always agree with the authors, it is an intellectual pleasure to read this "elementary quantum mechanics", possibly also as an introduction to Primas' *Chemistry, Quantum Mechanics and Reductionism* (Lecture Notes in Chemistry, vol. 24).

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