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A Review of: "The Basics of Theoretical and Computational Chemistry, by Bernd M. Rode, Thomas S. Hofer, and Michael D. Kugler"

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Book Review

The Basics of Theoretical and Computational Chemistry, by Bernd M. Rode, Thomas S. Hofer, and Michael D. Kugler, Wiley-VCH, 2000; ix + 183 p; $75.00, cloth. ISBN 3-527-31773-2

I start my review of this book at the end, or more precisely with the end of the book: its back cover. It shows the three authors on motorcycles, a feature I find to be a meaningful metaphor for the entire volume and so provides the framework for my comments.

As three individual riders, each need not be going in the same direction as the others, or as do two passengers in an automobile. As three riders, this parallels the situation between chemistry, physics, and mathematics (the first including biochemistry and chemical engineering, the last including computations as well), which can be symbiotic or can be totally indifferent to the others and their contemporary advances.

The book describes some contemporary methodologies in molecular modeling of biologically relevant species but relatively little about more conventional chemistry. Indeed, one of the very few molecules that is discussed in any detail (including an appendix of computational output) is misnamed. $(HO)_2SO$ is generally named sulfurous acid (or sulphurous acid), but never have I seen hyposulfuric acid, despite a computerized literature search for this alternative name.

Motorcycles are smaller than automobiles and as such generally enjoy higher fuel efficiency, economy, and "freedom of the road." The current volume is astonishingly slim and affordable, at least compared to other current books on the subject. The authors have also taken the liberty of using the framework of linear algebra and vector spaces rather than that of differential equations and multivariable functions. The reviewer acknowledges the power of this approach but differs with the authors that this is easier to read by most (at least, American) undergraduates or members of the professoriate who want to learn about theory. In my more than 30 years of university teaching, I have known perilously few undergraduate (and graduate) students for whom I suspect the current book would have been a facile introduction

to the subject. This is not to say the subject is generally easy to learn. However, the new approach may well challenge professors as a teaching modality as well because of its unconventional approach and its pedagogical as well as scientific assumptions. The various chapters are accompanied by a short collection of questions that generally involve thinking about more than mathematical manipulations, and in turn more than computations. Nonetheless, this is a good book for those who are already knowledgeable about theoretical chemistry. Motorcycles offer the rider a different view of the road and scenery than automobiles.

Motorcycle riding can encourage aggressive behavior, recklessness, and self-endangerment; both the vehicles and their drivers are very often louder than automobiles. Motorcycles are also less safe than cars for the neophyte; they can tip over more easily and are more vulnerable in collisions. The authors tell the reader "how to deal with the majority of these qualitative [MO and VB] models [as] given in Fig. 4.1." Their pictorial assertion, and associated text, qualifies in that regard. The picture is a color photograph of a wastepaper basket filled with models of molecules and orbitals! As it is the authors' style of giving quotes, let me give a favorite quote of mine: "Of course what we're doing is wrong, but that doesn't make it defensible" (from a cartoon by Ziegler in the *New Yorker*, February 28, 1977, p. 26). The current authors are right in that orbitals, *per se*, do not exist, that they are mathematical and not real objects. However, my view is that the impression that can be received by some readers is a disservice to the practicing chemical community, for which the use of orbitals provide both qualitative understanding as well as numerical results. I consider the authors' attitude most unwise and unsafe; it collides, without apology, with the preference and prejudice of most practitioners, whether at the beginning level of learning quantum numbers or that of the seasoned scientific researcher.

Summarizing, it is clear that motorcycles are not my preferred conveyance nor will this book be my preferred text in theoretical chemistry. I leave it to the readers to decide its suitability for enhancing their research or classes.

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