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Book Review

Clark, Timorthy R. and Rainer B. K. The chemist's electronic book of orbitals, Springer-Verlag, Germany, 1999, 96 pages/softcover US $39.95, GBP 19.00 ISBN 3-540-63726-5

In 1973 Jorgensen and Salem published a book named "The organic chemist's book of orbitals" (ISBN 0-12-390250-9). For more than three and a half decades, this book served as a standard reference book for molecular orbitals of some simple organic molecules as it contains the wireframe plots of the molecular orbitals of 104 simple organic molecules calculated using semiempirical methods. Orbital energies calculated using the ab initio, MNDO/2, and extended Hückel methods are listed along with the plots. This book can also be used as a supplementary textbook for an upper-level undergraduate or graduate-level quantum chemistry course.

Clark and Koch have made a giant step forward by introducing "The chemist's electronic book of orbitals'. The book has four concise main chapters (Chapter 1 is the introduction). Chapter 2 covers linear combinations of atomic orbitals starting with H_2. Chapter 3 deals with larger molecules, Chapter 4 introduces reactions and Chapter 5 ends with elementary symmetry concepts. The book is easy to read, requiring only a very basic mathematical and quantum chemical background. It proceeds effortlessly to the most important part — the reactions in Chapter 4. The most important reaction types in organic chemistry are discussed including Lewis acid/base reactions, S_{N^2} reactions, selectivity, frontier molecular orbital theory, the nucleophilic oxirane ring-opening reaction, the Woodward-Hoffmann rules, electrocyclic reactions, cycloadditions, and sigmatropic rearrangements.

The most distinguished feature of this book, as its name implies, is however its companion compact disc (CD) containing an electronic version with many interactive figures and molecular orbitals in virtual reality modelins language (VRML) format. The VRML plots are platform-independent and, thus, can be used on a PC, a Mac, or a Unix workstation. Demonstration 1 shows a simple example of the interactive features of the book. One can drag two hydrogen atoms from 10 Å apart to 1 Å or closer and watch the evolution of the molecular orbitals and energy levels. Do the same thing for two helium atoms and one will understand easily why helium does not form a diatomic molecule. The differences between σ and π orbitals are also shown very clearly by the interactive Java features. Many keywords (such as HOMO, LUMO, LCAO) are linked to the glossary; thus, one can go back and forth between the main text and the glossary and try to understand these keywords quickly.

There are molecular orbitals for 167 simple organic molecules on the CD. These orbitals are produced using the AM1 method with optimized geometries. The orbitals are plotted in blue and red wireframe format with the molecules as black and white ball-and-stick models. Unlike in the Jorgensen and Salem book, all the VRML plots are interactive. One can move, rotate, magnify, and examine them in much more detail. The orbital energies, however, are not given.

The interactive book on the CD can be viewed on a Unix workstation. I tried it with a Silicon Graphics O2 running IRIX 6.3 without any problem. However, it did not work initially on my PC running Windows 98 and Windows NT 4.0 (Service Pack 5) using Microsoft Internet Explorer 5.0. I needed to download CosmoPlayer from cosmosoftware.com according to the instructions in Chapter 8 of the book. With Microsoft Internet Explorer 4.0, the CD can run without CosmoPlayer. Once running, it is an enjoyable interactive book to read.

The book will be of great value for an undergraduate physical chemistry course or a graduate-level quantum chemistry course. It is also a great reference book for computational chemists.

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