Book Reviews

Deciphering the Chemical Code. By Nicolaos D. Epiotis. VCH Publishers Inc., New York. 1996. xlvii + 933 pp. 16.5 × 24 cm. ISBN 1-56081-946-4. $89.95.

This is perhaps one of the most provocative presentations of chemistry to come along in decades. In a discipline in which there has been a profound narrowing of concepts down to the acceptance of bonds as either covalent or ionic, this book moves back the limits of focus to admit new ideas. Epiotis opens up the discussion to include startling new ideas of bond types, three in number. His T bonds relate to covalent bonds and the E bonds to ionic bonds, while his I bonds are entirely new, describing bonds in organometallics.

The author vigorously challenges the current theories. He begins with the premise that electron−electron repulsion is the critical attribute that distinguishes the various chemical systems. He points to incorrect conclusions from existing theories, showing that his concepts give accurate accounts of these problems and inconsistencies.

The book is a provocative, fresh breath of ideas that will appeal to those who by nature may be skeptical of conventional wisdom and who are looking for new, creative insights to replace the chemical dogmas that have been accepted unquestioningly.

The book may serve as a source of new ideas to those pursuing the definition of molecular structure for the purposes of relating molecules to biological function. In this era when we seek to define structures for topological, electrodynamic, and similarity considerations, a compilation like this could serve as a starting point for these efforts. It is a worthwhile book to read even for no other purpose than to clear away the cobwebs of conventional thought and to engender some exciting controversy.

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Computer-Aided Molecular Design. Theory and Applications. By Jean-Pierre Doucet and Jacques Weber. Academic Press Ltd., London. 1996. xix + 487 pp. 17.5 × 24.5 cm. ISBN 0-12-221285-1. $55.00.

This book is a unique attempt to produce a real *text* on the theory and applications of computer-aided molecular design (CAMD). The computational chemistry/molecular modeling field needs such a book as many academic institutions have added molecular modeling instruction to their curriculums. Indeed, *Computer-Aided Molecular Design. Theory and Applications* can be used in a classroom setting or by individuals wishing to learn the technology. Many of the current techniques of CAMD, including graphics, databases, force fields, dynamics, quantum chemistry, molecular similarity, pharmacophore mapping, and protein modeling, are explained with the level of detail that an advanced undergraduate or beginning graduate student can grasp. A nice presentation on distance geometry is especially appreciated. The fact that this book was written by a single pair of authors, rather than being a loose collection of contributed chapters, strengthens the overall presentation significantly by adding coherence absent in other texts.

Surprisingly, the authors have been able to produce this text without significant references to commercial software packages. This is an admirable achievement! Unfortunately this lack of allegiance to one of the major commercial packages will make much more difficult the writting of a companion workbook. This reviewer hopes that a workbook (or family of workbooks) is under consideration. A minor complaint should be recorded. In many places the language is awkward. The publisher should have assigned an editor to help the authors with this book.

In summary, this is a very useful reference and text for beginning and advanced researchers in molecular modeling. It should be strongly considered by instructors as a potential student text for academic or industrial courses in molecular modeling.

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