

Book Reviews

Das HMO-Modell und seine Anwendung. Grundlagen und Handhabung. EDGAR HEILBRONNER and HANS BOCK. Verlag Chemie, GmbH, Weinheim/Bergstrasse, Germany. 1968. xii + 404 pp. 17 × 24 cm. 39.80 German marks.

Given the proliferation of introductions to molecular orbital theory for organic chemists, hardly anyone would have predicted that it should be possible to write still another one, which would be completely novel and yet at the same time comprehensive and pedagogically effective. Well here it is.

The German paperback is the first volume of a three-volume set. The foundations and applications are described in the first volume, followed by 250 solved examples in the second, and tables of calculated and observed variables in the third. The novel features of Heilbronner and Bock's approach are apparent in the first chapter. They analyze there in some detail the motion of a particle in a one- and two-dimensional potential-free box. Thus are neatly introduced all the fundamental concepts—wave function, normalization, degeneracy, levels, configurations, spin states, and spectra. There is a unique description here of level and state correlation diagrams for a square box distorting to a rectangular one.

The succeeding chapters maintain the high level of interest, but at the same time manage most effectively to *teach* the reader all the essential features of the Hückel model and much more. I would here like to mention a selection of the original features. Throughout the book there is a reasoned and natural utilization of correlation and interaction diagrams. They appear first in the introductory chapter on the free-electron method. Then they reappear in the well-known separated atoms–united atom correlation diagram for homonuclear diatomics, are connected to an analysis of interacting systems *via* perturbation theory, are cleverly utilized in analysis of barriers to twisting around single and double bonds, and finally are applied to a description of electrocyclic reactions.

The Heilbronner–Bock volume also contains an extensive introduction to the applications of perturbation theory, which is superior to any I have seen elsewhere. It could, however, be better. M. J. S. Dewar has recently aptly termed chemistry as “an exercise in perturbation theory.” The judicious application of perturbation theory can produce strong qualitative arguments. The trouble is that hardly anyone teaches the subject in a useful manner. In introductory quantum mechanics courses it is all too easy for teacher and student to be seduced by the beauty of the mathematical apparatus and thus to avoid an understanding of “the physics of the situation.” (The very same problem occurs in the teaching of thermodynamics.) Even the quantum chemists who use perturbation theory successfully tend to overwhelm the reader with a welter of coefficients when the conclusion could just as well have been arrived at by applying some simple verbal arguments, soundly based on perturbation theory, about how orbitals really interact.

Recent years have seen a resurrection of interest in the σ system of molecules, long neglected at the expense of conjugated π -electron systems. One has mixed feelings about the past development of π -electron theory. On one hand, the field has been a fruitful testing ground for approximations and extensions. On the other hand, one feels that perhaps a lot of the work has been in the nature of mathematical games, with little concern for the realities of chemistry. Anyway, the newer textbooks are beginning to introduce people to σ -electron calculations. The present book begins in an interesting way with a discussion of the interhalogen compounds, proceeding to xenon compounds and a simplified all valence electron treatment of ethylene. My own preference would have included here an extended analysis of Walsh diagrams, which are mentioned briefly later on in the book. I also would have attached a discussion of the transformation between the completely delocalized symmetry-adapted molecular orbitals which are the end product of *ab initio* calculations and the semilocalized bonds that organic chemists use in their everyday thinking.

The book begins with a quotation of a 1938 page by Erich Hückel and ends with some repartee and a fable from less scientific but not less perceptive sources. I am sure that this volume will be shortly translated into English.

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Halides of the Second and Third Row Transition Metals. By J. H. CANTERFORD and R. COLTON, Department of Inorganic Chemistry, University of Melbourne, Parkville, Victoria, Australia. John Wiley and Sons, Inc., 605 Third Ave., New York, N. Y. 1968. xx + 409 pp. 15.5 × 23.5 cm. \$15.95.

As the title of this book indicates, it is a highly specialized volume, being devoted exclusively to the simple and complex halides and oxide halides of the second- and third-row transition metals. It is to be one of a series of three volumes, the other two being entitled “Halides of the First Row Transition Metals” (by the same authors) and “Halides of the Lanthanides and Actinides” (by D. Brown). The first three chapters of this volume review the chemistry of (1) fluorides, (2) chlorides, bromides, and iodides, and (3) cluster compounds, from points of view of preparation, structure, stability, chemical and thermodynamic properties, and bonding. These chapters make interesting reading. The remaining eight chapters consider the halides of the transition metals by periodic groups, starting with zirconium and hafnium, and continuing to silver and gold. (The three vertical rows of group VIII are considered separately.) In each chapter, the compounds are treated in order of decreasing oxidation states of the metals, and “within each oxidation state, the order is invariably fluorides, chlorides, bromides, and finally iodides.” As the authors indicate, this makes for monotonous reading, but allows one to locate needed information quickly. In fact, few people will wish to read these chapters, except to look up specific pieces of information. For this purpose, it should serve admirably. Much of the information is presented in tables and diagrams, and in many places, the authors comment on the adequacy and accuracy of the work or suggest research that is still to be done. This is not the case throughout, however, for one frequently finds such statements as “It is reported that . . .” with no evaluation of the report, or two divergent views are cited, with no comment as to which the authors of this book prefer, and the reason for their choice. Their purpose, no doubt, is to encourage the reader to consult the original literature and draw his own conclusions. The book is heavily documented, there being almost 2000 references. The bibliography is complete to the end of 1966, and some material has been added up to 1968. The subject index is very short but is adequate in view of the arrangement of the chapters. The lack of an author index is unfortunate, but is understandable since such an index would have to contain several thousand entries.

Although the authors state in their preface that this volume may serve as a basis for university courses in the chemistry of the second- and third-row transition metals, it seems to this reviewer that only the first three chapters are well fitted for that use. Those three, and the remainder, will be of reference value to persons working with transition metals, or with halides.

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