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Approximate Molecular Orbital Theory, by J. A. Pople and D. L. Beveridge. VIII+214 pages, New York: McGraw-Hill 1970.

This book is an account of the research of John Pople and his coworkers in the past five years on the CNDO and INDO methods. The title is well-chosen to distinguish the scope of this book from seemingly similar recent books on semiempirical methods. Indeed, it has to be regarded as a theoretical book which intends to bridge the gap between theoretician and experimentalist.

The concept is simple and powerful. It consists of only four chapters and two appendices. Chapter 1 gives the quantum-mechanical background. Chapter 2 rigorously develops the self-consistent molecular orbital theory. On this sound basis, the approximate molecular orbital theories CNDO, INDO and NDDO are introduced in Chapter 3. The final chapter which covers about half the book presents applications of approximate molecular orbital theory. Most of it is information about CNDO and INDO calculations of molecular geometries and electronic charge distributions of a large number of first-row and a few second-row molecules. But also spin-spin interaction problems are considered with regard to hyperfine coupling constants and spin density. The quantitative results of Pople's recent research on these topics is contained in the 32 tables and 11 figures of this chapter. The appendices consist of a FORTRAN IV computer program for CNDO and INDO calculations and the evaluation of one- and two-center integrals.

Comparatively little effort is spent on comparing these results with other work. Applications of CNDO, INDO or similar methods by other researchers are presented on two pages only. Although this seems regrettable from one point of view, it serves to preserve the homogeneity of the presentation.

We are sure that this book will be welcome by those who are interested in applications of the CNDO and similar methods and we recommend it to anybody who is interested in semiempirical methods on a sound theoretical basis.

K. Jug

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