

Hückel molecular orbital model

The HMO Model and its Application. Vol. 2: Problems with Solutions. Vol. 3: Tables of Hückel Molecular Orbitals. By E. Heilbronner and H. Bock. Translated by W. Martin and J. Anthony Rackstraw. Pp. viii+449 and viii+190. (Wiley-Interscience: London and New York; Verlag Chemie GmbH: Weinheim, 1976.) £15 and £9; \$33 and \$18.

THESE volumes complete Heilbronner and Bock's handbook on the Hückel molecular orbital model. Volume 1 set out the basic theory and techniques, and contained numerous problems; Volume 2, which is almost as long, contains only the solutions to those problems. Anyone who works through all the problems would acquire a very extensive knowledge of Hückel theory. I suspect, however, that this knowledge would be deficient in being rather mechanical, superficial and uncritical. It is typical, for example, that although the main text provides an adequate

general derivation of the pairing theorem, the associated problem requires the reader to prove that a crude approximate formula for Hückel energies also satisfies the theorem—a result of far less power and significance. Again, the authors provide a mechanical procedure for factorising a Hückel determinant with the help of the molecular symmetry. Not only is it mechanical; it is also unnecessarily laborious, since it involves a lengthy series of operations on the entire secular determinant. Not only that; it doesn't even work where there are degeneracies (try it for cyclopropenyl). Setting up the determinant directly in terms of symmetry-adapted functions is easier, more general, and more illuminating.

Hückel theory is well known to be a very poor approximation for many purposes. The authors point out some of its failings, but do not indicate how they may be overcome, even by providing a suitable reference. Examples are the failure to predict negative spin populations, and the false degeneracy of the second excited state of alternant hydrocarbons. These are both due to the failure of Hückel theory to take account of electron repulsion; however, in both cases a simple correction can

be made to improve the Hückel result.

The third volume contains tables of Hückel molecular orbital coefficients and derived quantities such as bond orders and atom-atom polarisabilities. It covers chains (up to 10 atoms), rings (up to 18 atoms), an assortment of alternant and non-alternant molecules with up to three rings, and the partial π systems obtained by removing one carbon atom from naphthalene, anthracene, phenanthrene, azulene and biphenylene. It is intended partly as an adjunct to the problems, many of which refer to the data in the tables; however, it is also more generally useful. On the other hand, when writing a Hückel molecular orbital programme is a straightforward undergraduate exercise it cannot be said that the need for such tables is very great.

In summary, the work cannot be regarded as a definitive treatise on Hückel theory: it omits too much. As an introduction it is reasonably thorough, although even here there are some omissions. A useful but not indispensable book. **A. J. Stone**

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Plasma in gas

Plasma Phenomena in Gas Discharges. By R. N. Franklin. (Oxford Engineering Science Series.) Pp. ix+249. (Clarendon; Oxford: Oxford University: London, 1976.) £15.

LECTURE courses spawn books as readily as the proverbial salmon spawning eggs. Unfortunately graduate courses and the books they gestate too frequently limit themselves to the particular interests of the lecturer. This would seem to be the rationale behind this scholarly but narrow book by Raoul N. Franklin.

The book is largely concerned with analysing the positive column and illustrating the diversity of plasma phenomena which can occur therein. Though these small scale, low current, experiments are of great importance in the historical development of plasma physics, they nevertheless represent a very small area in what is now a much wider experimental field.

In the first half of the book detailed solutions of radial equilibrium, of space-charge effects at walls and electrodes and of the influence of a magnetic field in a positive column are presented. The second half of the book rests a little uneasily on the first part and aims to describe the variety

of plasma phenomena that can be observed in gas discharges. It is largely, however, a catalogue of linear plasma waves, including electron plasma waves, ion waves, ionization waves, magnetosonic and 'whistler' waves and drift waves. As a description of wave phenomena in plasmas, it is a useful and reasonably comprehensive compendium, though at this level it must be compared with many excellent books on waves in plasmas. I would have been happier with more physical insight, discussion and interpretation of the equations used and results obtained, as opposed to the *ad hoc* writing down of equations, linearisation and solution of the resultant dispersion relations. As a wide catalogue and a clear analysis of waves in plasma it is useful. A helpful feature is the inclusion of comparisons with experiment whenever possible and a wide range of references to experimental work.

Though the editing can be faulted and the production is dull, the book is scholarly and precise. It is certainly a useful text for those working directly in gas discharges but of less value to the wider student of plasma physics.

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