

Hartree-Fock method

The Hartree-Fock Method for Atoms: A Numerical Approach. By C. Froese Fischer. Pp. 308. (Wiley Interscience: London and New York, 1977.) £17.20; \$29.

THE Hartree-Fock (HF) method means different things to different people. The one point in common is that a wave function Φ for a many-particle system is constructed from anti-symmetrised products of one-particle functions ϕ , and that the latter are fully optimised. In many-body theory, as used in nuclear and solid-state calculations, Φ is taken to be a single determinant.

In applications of HF theory to non-relativistic atomic structure calculations, which is the subject of this book, the condition is invariably imposed that Φ must be an eigen function of total spin and total orbital angular momentum operators. In all but the simplest cases, this condition implies that Φ must be a linear combination of several determinants. The HF approximation for atoms is sometimes taken to imply the restriction that Φ is constructed

from functions ϕ , all belonging to the same configuration (although the exact meaning of this statement is not always clear, as is illustrated by Froese Fischer's discussion of the $1s2s^1S$ state). In 1939, Hartree, Hartree and Swirles showed that this restriction need not be made. They introduced the multi-configuration method (MCHF), which has been used extensively in recent years, and provides one of the most powerful known methods for calculating accurate atomic wave functions. A great deal of skill has been devoted to the development of the numerical and computational techniques required for this work, and they are clearly described in this book, which puts particular emphasis on methods using numerical integration of the equations (as opposed to those using expansions in terms of basis functions).

The book gives a lucid account of the foundations of atomic HF theory, a detailed account for the specialist of modern MCHF work, and concludes with a useful discussion of available computer programs for atomic structure calculations.

M. J. Seaton

M. J. Seaton is Professor of Physics at University College, London, UK

Dielectric relaxation

Dielectric Spectroscopy of Polymers. By Peter Hedvig. Pp. 430. (Adam Hilger: Bristol; Akademiai Kiado: Budapest, 1977.) £17.50.

IN the past decade, an attempt has been made in many laboratories to unify the study of the dielectric, mechanical and nuclear magnetic resonance (NMR) relaxations in solid polymers, into a coherent spectroscopy. The underlying desire in this attempt was to put forward an interpretation on the molecular level for the observed relaxations. Although such a unified approach has not yet been achieved, Peter Hedvig's book is an excellent up-to-date review on efforts towards this aim.

This first two chapters deal in a concise and precise way with the principles of dielectric spectroscopy and structural transitions and molecular mobilities in solid polymers. Transitions in the glassy state involving local molecular motion are discussed using the potential barrier theory. Cryogenic relaxation phenomena are presented together with the molecular level interpretation. Transitions in the crystalline phase involving defects and orientation effects are discussed, well illustrated and supported by an extensive list of references.

These are followed by three chapters

which present both the experimental techniques and results of dielectric, mechanical and NMR spectroscopies together with dilatometry and differential thermal analysis. The depolarisation technique and the new time domain method (Fourier method) are presented in detail. Dielectric spectra of both pure polymers and polymer compounds are examined both from the chemical structural point of view as well as from the point of view of 'physical' phenomena such as plasticisers and filler effects.

In the last two chapters the study of crosslinking and ageing processes by dielectric spectroscopy is presented. These chapters are unique and original in the literature, and are of special interest to those involved in the technological aspects of dielectric spectroscopy of solid polymers.

In the Appendix the relaxation maps of 31 polymers are presented. This collection is of value to the experimentalist working in dielectric and mechanical spectroscopy fields.

All in all, the book is informative, well balanced, well illustrated and has few errors. It is strongly recommended both for the experimentalist in the field of dielectric relaxation as well as for the advanced student of that domain.

Shimon Reich

Shimon Reich is a Senior Scientist in the Polymer Department at the Weizmann Institute of Science, Rehovot, Israel.

Metabolic yearbook

The Year in Metabolism, 1975-1976. Edited by Norbert Freinkel. Pp. 353. (Plenum Medical: New York and London, 1977.) \$27.

THIS is the first of a new series of annual publications in which the previous year's developments in selected broad areas of metabolism related to human disease are reviewed. The following topics were chosen: hormone receptors, cyclic nucleotides and control of cell function; diabetes mellitus; glucagon; body fuel metabolism; obesity; lipid and protein metabolism; amino and mono amino organic acids; purine and pyrimidine metabolism; vitamins and minerals; urinary stones; the metabolic aspects of ethanol.

The topics chosen are appropriate because there is updating to be done in each case, and in some cases the authors have had to be selective within their chosen field; for example, chapter 9, "What's New—Vitamins and Minerals", deals only with vitamins C and D, although the author indicates that there may be changes in the future.

I found little of substance to criticise in this book but I am left in some doubt as to its most appropriate target. The honours student in biochemistry will find it much too clinically orientated, and the undergraduate medical student as well as almost all postgraduate medical students will find it much too detailed in a few narrow spheres. It is, in my opinion, a book for specialist metabolic physicians and medical research workers, as well as others who wish to read an up-to-date account of one of the topics covered. It will be invaluable for them.

The real test of this publication's success will be the extent to which the impetus which has brought it into being can be maintained. This implies that each chapter should be re-written for each new edition. If this can be done, it may well provide a needed intermediate between the very condensed but comprehensive publications of the *Annual Reviews* type, and several very good, well-edited and up-to-date large textbooks on the subject, with all of which it will be in competition.

R. W. E. Watts

R. W. E. Watts is Head of the Division of Inherited Metabolic Diseases at the MRC Clinical Research Centre, Harrow, UK.