Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333, Jay Street, Brooklyn 1, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

The Calculation of Atomic Structures. By D. R. HARTREE. New York: Wiley; London: Chapman and Hall. 1957. Price $5.00; 40*s*.

No crystallographer needs to be told of Hartree's work. His calculations of atomic structure have provided the basis for almost all quantitative calculations of X-ray diffraction, through their use in the determination of atomic scattering factors. From his first papers in 1923, Hartree was interested in the crystallographic applications of atomic theory, and he had made a valiant effort to find the charge distributions in the atoms, using the older methods of Bohr's theory, before wave mechanics was developed in 1926. With the discovery of Schrödinger's equation, he was in a unique position to apply wavemechanical methods to a determination of the wave functions of atoms, in terms of the one-electron central-field approximation. These results were applied to crystallographic problems from the beginning: in the same year, 1928, in which the first calculations by the self-consistent-field method appeared, there was also the classic paper of James, Waller & Hartree, in which Hartree's calculations of the atomic scattering factors of sodium and chlorine made it possible to test the Debye temperature factor quantitatively, and to demonstrate the existence of the zero-point energy in rock salt. Other calculations of Hartree relating to X-ray problems, in particular his paper with Waller which elucidated the relation of Compton scattering to the intensity of total scattering of X-rays, are classic contributions to the field.

All of these applications, however, are secondary to the major contribution which Hartree had made to physics: the development of a practical, usable method of approximating to the wave functions of complicated atoms. The method of the self-consistent field, and its extension to the case where exchange is included, usually known as the Hartree–Fock method, give us approximate wave functions for the atoms which have errors in total energy of only a fraction of 1%, which give both X-ray and optical ionization potentials with relatively small error, and which give the most accurate estimates which we have of the charge densities in an atom. The peculiar importance of Hartree's contribution lies in the fact that, in a period in the development of physics when most theoreticians were content to use the crudest numerical approximations to illustrate the most elaborate and abstruse theories, Hartree has steadily pursued the more modest, but in many ways more valuable, aim of keeping to simple theories, but working them out as accurately as possible.

This little book (181 pages), developed from a series of lectures given both at Haverford College and at Princeton University in 1955, gives a full account of Hartree's methods of atomic calculation, and of many of the results obtained with it. It combines two aims: to explain atomic theory to the general reader with knowledge of wave mechanics, and to go into the details of the calculations fully enough to be useful to the expert who wishes to make calculations himself. Both of these aims are excellently fulfilled. The general discussion of atomic theory is necessarily brief, but it is clear, and very useful to a student. It does not go very far into advanced multiplet theory; it stops with the diagonal sum method, but that is all that is needed for the applications which are made. Naturally the greatest value of the book is in its excellent discussion of the methods of actually carrying out the calculations of atomic structures by the methods of the self-consistent field. The numerical methods, and the general ideas behind the calculations, are brought out very clearly. A chapter on the scaling of atomic wave functions, their change in going from one atom to another, is largely new material, and should be particularly useful to those who are trying to estimate the wave functions of atoms for which calculations have not been carried out. Unfortunately, there are many of these. Hartree himself, and his father, the late W. Hartree, have both been very energetic in carrying through calculations of many atoms, and many other workers have contributed to the field, but there are still many more atoms for which calculations have not been made than for which they have. This book may well stimulate new work in the field, and make the task of anyone who takes up the problem without previous experience much easier. It should be read by everyone interested in atomic theory.

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Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

The Powder Method in X-ray Crystallography. By L. V. AZAROFF and MARTIN J. BUERGER. Pp. xv+342 with many figs. New York; Toronto; London: Mc-Graw-Hill. 1958. Price $8·75; 68*s*.

X-ray Crystal Structure. By D. MCLACHLAN, Jr. Pp. xiii+416 with many figs. New York; Toronto; London: McGraw-Hill. 1957. Price $15·00; £5.16.6*d*.