

Book Reviews

Gas Chromatography. A. I. M. Keulemans. Reinhold, New York, 1957. xix + 217 pp. Illus. \$7.50.

In the last few years, the technique of gas chromatography—that is, the chromatography of volatile substances in which a permanent gas is used as the moving phase—has grown very rapidly. It is becoming standard in many laboratories, both industrial and academic, as a means of analysis of volatile mixtures. Of late, several manufacturers of scientific apparatus have produced gas chromatography machines that join the ranks of the magic black boxes which form the physical analyst's stock-in-trade.

In view of the rapid rate of growth of the subject at present, A. I. M. Keulemans' book should be very valuable. After an initial chapter in which gas chromatography is compared with similar analytic methods, there is a chapter outlining the apparatus used in its technique and the way in which it will perform both qualitative and quantitative analysis. Several examples from the published literature are quoted, displaying practical analyses. In the third chapter, the components of the apparatus are described in greater detail. These three chapters give the basic outline of the subject. The book then continues in greater detail, presenting a theory of the chromatographic process, which is developed into a discussion of the design, construction, and performance of gas-chromatographic columns. The discussion is extensively illustrated from practice and gives much information which makes it possible to use the technique in the most effective manner.

The book is a textbook rather than a comprehensive treatise. The material discussed has been selected with regard to its importance and is particularly valuable to those who use commercial instruments. Nine-tenths of the book is devoted to the gas-liquid partition chromatography of Martin and James, while there is only a short section on gas-solid adsorption chromatography, which is at present rather overshadowed by the other. The treatment of the theory of the column and its operation is much more detailed than the description of

the apparatus. This is inevitable, since the design of the apparatus is so diverse and is developing so rapidly, whereas the theory will, it is presumed, remain invariable.

Keulemans is associated with the Shell Oil Company, whose work in this field is outstanding. He has drawn extensively on Shell work, and in places where views might be controversial, he voices those of Shell workers. The accent throughout is on the use of the technique in the oil industry. Certainly, to date, the method has been of the greatest value in this industry, and the oil companies have done the greater part of the development. However, it should be emphasized that the technique is of general application to anything volatile, and this book should be of great interest to anyone who feels that he should know about the analysis of any volatile mixture.

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The Calculation of Atomic Structures.

Based on lectures given under the auspices of the William Pyle Fund of Haverford College, 1955. Douglas R. Hartree. Wiley, New York; Chapman & Hall, London, 1957. 181 pp. Illus. \$5.

This book has been written in response to a recent revival of interest in the results of calculations of atomic structures and of methods of carrying out such calculations. This interest has been quickened by the rapid development of automatic digital computing machines and methods, which will make atomic structure calculations easily practicable on a much more generous scale than before and over a much greater range of cases (notably, for heavier atoms). The book "is intended for those who want to know about, or to carry out, quantitative calculations of atomic structure" to the degree of approximation embodied in wave functions of the "self-consistent field" type, using the methods developed by Hartree and Fock. The book makes no attempt to deal with the more detailed features of atomic energy states, such as multi-

plet structure, hyperfine structure, or the effects of external fields.

The first three chapters comprise a brief introduction, a discussion of the application of the variation principle to atomic structure, and the derivation of basic equations for the computation of atomic wave functions and energies in the self-consistent field approximation for closed-shell atomic states ("configurations of complete groups").

Chapters 4 and 5 describe, in considerable detail, numerical procedures for the solution of the self-consistent field problem in the closed-shell case, and their application. The book as a whole, and these how-to-do-it chapters in particular, for the first time bring together in one convenient place the fruits of the author's long experience in hand computations with the self-consistent field method. All the most recent improvements in technique through 1956 are included. Chapter 6 extends the discussion of chapters 3 through 5 to configurations comprising incomplete groups. The possibility that modified techniques or approaches may be more suitable in digital computer programming is considered very briefly, but actual methods of implementation of machine computations, already under way in two or three places, are not discussed.

Chapter 7 is designed to fill the need for the best possible procedures for interpolation between cases of atoms or ions for which self-consistent field calculations have been made. (For example, if self-consistent field wave functions were known for Si and S but not for P, one might estimate those for the latter by interpolation.) At the present time, such interpolation procedures are needed because not much more than a sampling of all cases of interest has been carried out, except for the lightest atoms. They are needed for either or both of two reasons: (i) for the calculation of atomic properties, in lieu of wave functions computed directly by the self-consistent field method; (ii) for use as initial estimates in making self-consistent field calculation, since the effort of making such a calculation can thereby be greatly reduced. Various useful curves, diagrams, and (in Appendix 2) tables are included.

Chapter 8 sets forth methods for computing the energies, in particular of levels differing in the number or state of excitation of outer electrons, when self-consistent field wave functions are known. Chapter 9 briefly surveys how the self-consistent field calculations may be extended to take account of relativistic effects.

Chapter 10 is an up-to-date critical brief review of methods of obtaining better approximations to atomic wave