BOOK REVIEWS

Organic Chemistry, 4th Edition

Stanley H. Pine, James B. Hendrickson, Donald J. Cram, and *George S. Hammond,* McGraw-Hill Book Co., NY, 1980. xiv + 1039 pp. Figs. and tables. 19 × 24 cm. $27.50.

This text represents a thorough rewriting of the previous edition, which appeared in 1970. Although it no longer retains the organizational divisions of Structure, Dynamics, and Special Topics carried through the first three editions, the flow of topics is largely unchanged. The present edition is comprised of 21 chapters, starting with 5 chapters covering topics on history, classes of compounds, nomenclature, functional groups, bonding, stereochemistry, and spectroscopy. Chapter 6 presents an introductory treatment of structure, reactivity, and organic transformations, and this is followed by 7 chapters covering the principal mechanistic categories. Chapter 14 deals with organic synthesis and the remaining 7 chapters are devoted to the specialized topics of carbohydrates, nucleosides, amino acids, peptides, proteins, lipids, free radicals, molecular rearrangements, natural and synthetic polymers, photochemistry, and organic electrochemistry. Each chapter contains numerous exemplary questions interspersed throughout the text and supplementary problems at the end. Answers to representative questions are not given. The book concludes with a very thorough index. The nearly 1300 pages of the previous edition have been cut by over 200 pages. The use of red ink in the previous edition to highlight points of interest has been abandoned. In all, the book is attractively printed and is easily read. It was obviously carefully proofread prior to being printed.

The authors indicate in the preface that the first 13 chapters are designed to provide the student with a good introduction and the remaining 8 chapters represent applications of fundamental principles to topics of special interest. Whether this division would work out conveniently into a two-semester presentation would probably depend upon the instructor's goals and interests. Because the first part of the text retains the general organizational development of topcs found in the previous edition, it has the same pedagogical limitations; i.e., those who object to a rather extensive build-up of what might be considered background information before chemical reactions are seriously dealt with will find the present edition only slightly improved over the previous one. On the other hand, the early treatment of functional groups, nomenclature, and spectroscopy offers some advantages to the students in the associated laboratory class.

A question quite apart from how a text is organized is that of what topics are included. In this regard the authors have effectively interwoven subjects of current practical interest with those of a more academic nature, and the result is a fairly comprehensive coverage. As befits an introductory text, there does not appear to be a disproportionately large amount of attention centered on any single topic.

In all, this new edition represents a major addition to the growing list of introductory texts available to teachers and students of organic chemistry. It will certainly find enthusiastic users among those who favor its particular organizational approach.

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Handbook of Practical Organic Microanalysis

S. Bance, Ellis Horwood Ltd., Chichester, 1980. 206 pp. Figs. and tables. 15.5 × 23.5 cm. $58.95.

The title of this book brings to mind the confusion which now exists between the terms describing the ancient art of "organic microanalysis" and the rapidly growing field of "trace organic analysis." The latter actually does not encompass "analysis" at all and should more properly be referred to as "trace organic determinations." Quantitative organic microanalysis never played a very important part in the undergraduate curriculum and today has all but completely disappeared in favor of more glamorous subjects. The determination of the elemental composition of organic compounds ("CHNOX" analysis) continues to be an all important tool of the synthetic and natural products chemists, but most receive these numerical results "like magic" from the "microanalysis laboratory" with little concern for the experimental design employed.

The author, a recently retired industrial chemist with 35 years of microanalysis experience, has effectively reviewed the field in a short, well-written handbook containing a wealth of experimental details. Most of the procedures discussed involve classical glassware rather than modern instrumentation, but many of these are still very widely used. The 24 chapters are dedicated to the following elements (among others) and groups: C, H, N, O, Cl, Br, I, F, S, P, As, Sb, B, Si, H_2O, alkoxyl, N-alkyl, acetyl. The book can be recommended highly as a source book for anyone interested in doing or teaching organic microanalysis, but in 1981 this probably does not represent very many chemists.

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Numerical Methods in Chemistry

K. Jeffrey Johnson, Marcel Dekker, New York, 1980. ix + 503 pp. Figs. and tables. 18.5 × 26 cm. $29.50.

In this unique text, numerical methods and computer programming are used as tools to solve problems encountered by serious undergraduate majors, graduate students, and researchers. A working knowledge of calculus and computer programming is assumed although the author reviews Fortran in the first chapter. The author adheres to standard Fortran except for a very few cases which he points out to the reader. Such careful attention to detail makes this text very readable and usable.

The author takes a methodical approach to each new chemical problem. In stepwise fashion he (1) introduces the problem, (2) discusses how the problem is solved numerically, (3) lists a sample execution of the program written to solve the problem, (4) lists the program, and (5) discusses the characteristics and special features of the program. In other words, the author provides an excellent model of problem solving which the student can and should emulate.

Each program is carefully documented internally, and most importantly, the programs work as they are listed. The reviewer tried some of the programs exactly as they are shown in the text, on a Honeywell-Xerox Sigma-9, and each program tried ran without modification or correction.

The problem sets given at the end of the chapters require application of techniques covered in the chapter and are challenging. Throughout each chapter, and in the problem sets, bibliographic references are cited so that the student has ready access to chemical information needed as background to understand and solve the problems.

Topics of increasing complexity from the standpoint of numerical analysis programming are dealt with progressively. In chapter two, for example, nine programs are used to teach the application of closed-form algorithms to chemical problem solving. Chemical topics covered include simulation of a kinetic system, calculation of reversible electrode potential, calculation and plot of the radial distribution function for hydrogen-like atoms, calculation and display of electron density contour plots, etc.

The third chapter deals with finding roots of equations or systems of simultaneous equations. Iterative techniques used in the Newton-Raphson and binary bisection methods are applied to such problems as "particle in a box" and gas phase equilibria. Linear and nonlinear systems of equations are solved in chapter four using Cramer's rule, the Gauss-Seidel method, and elimination methods applied to heterogeneous and gas-phase equilibria problems.

Regression analysis, covered in chapter five, is applied to a variety of chemical problems, and the trapezoidal rule, Simpson's rule, Cotes formulas, Gaussian quadrature, and the Monte-Carlo method are used to approximate integrals in chapter six. Euler's method, the Runge-Kutta method and the predictor-corrector method provide students with techniques to solve differential equations in chapter seven. Chapter eight is given to determining eigenvalues and eigenvectors of Hermitian matrices applied to systems such as three-spin proton NMR and Hückel molecular orbitals.

The last chapter contains a number of different topics. Most useful to the purpose of this text is the discussion of graphics. The brief review of computer applications to instruction and information science which follows seems out of place with respect to the purpose of the text, but the bibliographic references are excellent. It would seem that these topics will be of much more interest to

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