Book Reviews

Theory of Molecular Fluids. Volume 1. Fundamentals. By C. G. Gray (University of Guelph) and K. E. Gubbins (Cornell University). The Clarendon Press, Oxford University Press: New York. 1984. xiv + 626 pp. $79.00. ISBN 0-19-855602-0.

This is the first of two volumes devoted to theory of molecular liquids such as nitrogen and water. The recent advances in this field seem not to have excited the general chemistry community as much as the theory of atomic fluids did a decade earlier, yet molecular liquids are of vastly greater importance to chemistry and, as the authors carefully point out, there are new effects and complications in molecular liquids which have no analogue in liquid argon. Orientational correlations between molecules and new kinds of phase transitions are perhaps the most obvious examples.

Gray and Gubbins treat carefully the classical statistical mechanics of equilibrium, "non-critical fluid phases of small, nearly rigid molecules". This first volume seems to be setting the scene for the second volume on applications. It contains exquisitely detailed chapters on intermolecular forces, the basic statistical mechanics of correlation functions in pure liquids and mixtures, perturbation theories for both spherical and nonspherical reference potentials, and integral equation methods for molecular liquids. More than one-quarter of the volume is devoted to appendices covering everything one wants—and genuinely needs, in this field—to know about spherical harmonics, tensors, rotation matrices, and Clebsch–Gordan coefficients.

This is an outstanding reference work and it contains clear, in some cases unique, discussions of the pivotal mathematical developments in the field, for example, the Wiener–Hopf factorization method for solving the Ornstein–Zernike integral equation. It is surprising perhaps that only 8 pages are devoted to results obtained from interaction site models (ISM) of molecular liquids, which have had a large impact on the field, although the authors may be saving these topics for the second volume. However, it should be noted that this first volume does include some very recent and important derivations and applications (e.g., water) of ISM theories.

New workers in the field may find the extremely thorough discussions of forces and correlation functions in molecular liquids too detailed, and may benefit from the less complete, more instructive accounts in recent textbooks such as H. L. Friedman's "Course in Statistical Mechanics" (Prentice-Hall, New Jersey, 1985). The second volume of "Theory of Molecular Liquids" promises chapters on the thermodynamics and structure of pure liquids and mixtures, dielectric properties, and spectroscopic properties, and it is awaited eagerly.

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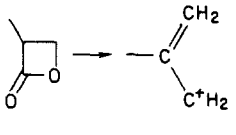
Multidimensional Pharmacochemistry: Design of Safer Drugs. By Peter P. Mager (Karl Marx University, Leipzig, GDR). Academic Press, Inc.: New York. 1984. xiv + 418 pp. $89.00. ISBN 0-12-465020-1.

This book is primarily devoted to multivariate statistics and data analysis as it applies to pharmacological, medicinal, and toxicological data. The discussion of multivariate statistics is limited largely to those techniques developed by the author.

The introductory chapter entitled Some Aspects of Medicinal Chemistry Today is intended as an introduction but is often little more than an editorial statement. The second chapter, Biochemical Pharmacological Design, deals with concepts relating to the behavior of drugs in biosystems. Thus, the focus is on pharmacokinetics, drug metabolism, and drug–receptor interactions. Unfortunately, this discussion is disjointed and often too simplistic and the author makes too many unwarranted generalizations. The chapter also contains a number of factual errors. For example, in a discussion of "most important reactions of phase I metabolism", the author gives the following as one example:



In another section the author incorrectly refers to the metabolic activation of the anticancer drug cyclophosphamide by phosphates (sic). Several structures are wrong, e.g., the mesoionic anticonvulsant on p 11, the imidazole H_2 antagonist on p 49, and the propam structure on p 57. The author uses antiquated or unorthodox terms such as "trojan horse carrier" and "selectophore". This 53-page chapter is of limited value and fails to develop any consistent theme.

Chapter 3, Underlying Theory of Multivariate Statistics, describes the general structure of the integrated multivariate statistical model MASCA (multivariate structure–activity analysis in combination with the multivariate bioassay) developed by the author. The author contrasts MASCA with univariate and other multivariate approaches. Chapter 4, Multivariate Bioassay, describes probabilistic principal component analysis, PRINCO, multivariate variance analysis, MANOVA, multivariate correlation and regression analysis, KANORA, multivariate covariance analysis, MACOVA, and multivariate autocorrelation, MARA. Chapter 5 gives a demonstration of the methods applied to the MASCA model. Chapter 6 gives a very weak discussion of "synthetic design", a very brief discussion of "molecular structure coding", and a more extended discussion of electronic, steric, and lipophilic substituent constants. Chapter 7, The Multivariate Quantitative Structure–Activity Relationship, is divided into sections dealing with the "traditional approach" (Free-Wilson analysis and Hansch approach), principal component regression analysis, overall-response parameter analysis, KANORA applied to QSAR, generalized parabolic model, and grouped observations (branching in QSAR). The final chapter gives a brief overview of future perspectives.

The 663 references (ca. 15% are P. P. Mager citations) are collected at the end. There are a few 1983 references and the remainder are 1982 and earlier. The book has a 16-page index.

The author stated in the preface that the book tries to bridge the gap between a cookbook of multivariate statistics and a minimum of mathematical background and a book on modern statistical theory. The book, to an extent, does accomplish that goal, although a significant mathematical background is required. The strength of the book lies in the detailed analysis of the integrated multivariate statistical model, MASCA, developed by the author. The weakness of the book lies in the nonmathematical discussions of drug design, drug metabolism, etc.

This book can be recommended to those individuals who wish to use multidimensional statistics to analyze biological data. The book is *not* recommended to those individuals seeking a book on the principles of drug design or the design of safer drugs unless they plan to use multivariate statistics to analyze data.

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Mass Spectrometry in Environmental Sciences. Edited by F. W. Karasek (University of Waterloo), O. Hutzinger (University of Bayreuth), and S. Safe (University of Guelph). Plenum Press: New York. 1985. xix + 578 pp. $75.00. ISBN 0-306-41552-6.

Seven chapters are devoted to instrumentation and techniques. Two chapters review air and water pollution, respectively. Each of the remaining 17 chapters relates to a specific class of chemical. Only 24 of the 1416 articles cited by the various authors were published later than 1981. This is by no means an up-to-the-minute dissertation, yet it is generously peppered with useful information.

The chapters on methodology range from superficial to superfluous. Comparatively little detail is given for the most widely-used techniques, while a disproportionate number of pages was allocated for descriptions of more esoteric methods. The discussions of water and air pollution are particularly disappointing. The former is largely restricted to the genesis of the EPA's Master Analytical Scheme, while the latter devotes considerable space to obsolete techniques. The remaining chapters, which constitute the bulk of the book, are truly invaluable to the practising environmental analyst. They cover such topics as polycyclic aromatic hydrocarbons, halocarbons (mostly of historical value), polychlorinated biphenyls and related compounds (2 chapters), phthalates and other plasticizers, organometallic compounds, nitrosamines, pheromones, and pesticides (8 chapters). A final chapter is devoted to miscellaneous synthetic and natural toxins. Most of these monographs introduce the reader to the subject, provide sample mass spectra, discuss fragmentation mechanisms, outline techniques of analysis, and address potential pitfalls and problems.

An index to some 200 mass spectral line diagrams is contained in an appendix. The subject index is adequate, though not comprehensive. There is no author index.

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