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Book reviews

Czerminski, J., Iwasiewicz, A., Paszek, Z., Sikorski, A. (1990) Statistical Methods in Applied Chemistry. Elsevier, Amsterdam Oxford New York Tokyo, and Polish Scientific Publishers, Warsaw, pp. XVIII + 493

The mathematical elaboration of the results of chemical measurements is usually considered as a topic lying outside the scope of traditional theoretical chemistry. As a consequence of this, scientists declaring themselves as theoretical chemists often have little or no interest in such kinds of approaches. Yet, the application of statistics to chemistry is not only of paramount importance for experimentalists and chemists performing routine measurements, but also provides challenging and mathematically nontrivial open problems.

This book written by a group of Polish chemists-statisticians may be used as an introduction to this particular field of applied mathematics. Although the book is practice-oriented with a large number of examples (from the fields of analytical, physical, industrial and environmental chemistry), its mathematical level is sufficiently high to satisfy theoretical chemists.

The authors follow a traditional pattern. Chapter 1 outlines the basic notions of random variables, probability theory, and statistics. Chapter 2 deals with the estimation of distribution parameters using samples. Chapters 3 and 4 are devoted to testing of statistical hypotheses. Chapter 5 considers the problems of correlation and regression. Some hints for practical work are collected in Chap. 6, followed by some full-length examples (Chap. 7). The book ends with a compendium of statistical tables and computer programs (written in Turbo Pascal).

In comparison with other treatises on statistics applied to chemistry the present book offers a not too rigorous and orthodox, yet theoretically sound approach; the theory is well counterbalanced with pertinently chosen real-life chemical examples.

The authors did their best to make the reader think statistically and not only to learn how to mechanically perform certain statistical recipes. In this respect a quotation is appropriate (p. 229): "*Just as much as otherwise effective anti-rheumatic treatment with radioactive baths can be the death of a patient with latent cancer, so can computerized mathematics become the grave of philosophy and creative thought.*"

The "Statistical Methods in Applied Chemistry" will be of great value for all those intending to master both the theory and the practice of data elaboration in chemistry.

Ivan Gutman, Kragujevac, Yugoslavia

Webster B (1990) Chemical Bonding Theory. Oxford, Blackwell. 297 pages, £14.95

A serious theory of the chemical bond can only be based on quantum mechanics and most textbooks in this field that I know of start hence with the Schrödinger equation and try to deduce valence theory from it. This involves some rather difficult steps, that one may go in a more or less rigorous way, borrowing more or less concepts from chemical experience. A reader who does not want to become a theorist, but who wants to get only some qualitative insight into theory is often horrified by the mathematics and physics required for a somewhat rigorous theory.

The present text follows different lines. Concepts based on chemical experience are from the very beginning regarded as equally legitimate as those coming from quantum theory. The author insists,

e.g., that his readers should first learn to draw Lewis double-dot formulae and to apply the Gillespie–Nyholm model before being introduced to the concept of atomic and molecular orbitals. Very little mathematics is needed and instead many pictorial illustrations are given, including contour plots of MOs obtained from *ab-initio* calculations. The relation to experimental methods or results is pointed out whenever this is appropriate. Less space is devoted to conjugated π-electrons than one is accustomed to from other textbooks, but one reads something about puckered rings and there is a rather detailed chapter on complex ions, as well as a short consideration of molecular attractions.

The presentation is appealing and from the didactic point of view this is a good textbook. The price is such that a student can afford to buy it.

The pragmatic attitude of this book necessarily implies a trend to oversimplifications. A clear distinction between rigorous concepts and heuristic models is seldom made. The presentation of MO theory is so rudimentary that the reader has not even a chance to realize the limitations of the MO model. Some parts, such as Sect. 6.5.1 or the Hellmann–Feynman theorem and the Berlin model are even misleading.

I can recommend this textbook to beginners with little mathematical or physical background or to experimental chemists who want to gain some basic idea of theory. For individuals who want to work in theory, a more critical attitude is necessary from the very beginning.

W. Kutzelnigg, Bochum

Announcement

24th Annual Quantum Theory Conference

This conference will be held in St. Peter Port, Guernsey, Channel Islands from September 30th to October 3rd, 1991.

The topic overlaps completely with the scope of this journal and also encourages contributions from physicists and mathematicians from which theoretical chemists might benefit.

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