

based approach to understand the interaction of aluminum ions with smectite clay. The studies described by Vivit, Thomas, and Laboriau have only recently become possible because of the introduction of probes fabricated with aluminum-free material, which reduces baseline roll due to acoustic ringing.

The third section of the text is entitled Nutrient and Natural Organic Matter (NOM) Cycling in the Environment. It focuses on research exploring phosphorus and nitrogen cycling in the environment, using either solid-state or solution NMR to investigate the structure of NOM under nondegradative conditions. Most of the NOM studies reported in this text utilized ^{31}P or ^{15}N NMR, as organic oxygen or sulfur is not amenable to either solution or solid-state NMR. The studies on NOM research presented in this section include P in organic wastes and fertilizers, the chemical characterization of nitrogen in plant composts and humic materials, and ^{13}C CP/MAS NMR studies of organic carbon in aquatic sediments and soil with low carbon content.

Each section of the text contains an overview chapter, which provides the reader with the necessary background to understand how NMR has advanced research in a particular area. The overview chapters promote continuity, which is often a problem with multi-authored texts. The final chapter of this book summarizes a panel discussion held at the end of the symposium NMR Spectroscopy in Environmental Science and Technology that was presented at the National ACS Meeting in Denver, Colorado, in 1993. Evidently, the symposium and panel discussion played a pivotal role in the development of this text. My overall opinion of the text is favorable. The references in the text are current and complete. The scientific level of the text is high. Clearly, this book will be a useful reference for chemists who require a basic knowledge of NMR for environmental systems or environmental engineers who seek to incorporate NMR techniques into their research.

Barry K. Lavine, *Clarkson University*

JA9755727

S0002-7863(97)05572-8

X-Ray Charge Densities and Chemical Bonding. IUCr Texts on Crystallography 4. By Philip Coppens (State University of New York at Buffalo). Oxford University Press: New York. 1997. xiii + 358 p. \$85.00. ISBN 0-19-509823-4.

This book has been eagerly awaited by those active in the field specified in the title. The author is well-known for his seminal contributions to the subject as well as his clear, lucid, and pedagogical lectures and writings. This book fulfills that expectation. But it is not just a monograph for those in the field. I would recommend it as a textbook for a graduate level course as well as supplemental reading for an undergraduate course in crystallography. Some exercises are included as well as a large number of references. Importantly it can be used for self-study by nonspecialists, e.g., a chemist who wants to be able to use the concepts and results from electron density studies in their own work.

But what is meant by X-ray charge densities? One is aware that in crystallographic structure determinations the scattered data are fit in a least-squares sense to a superposition of spherical atomic form factors situated at the atomic centers. The residuals are the remaining electron density as well as the errors. As quoted in the preface, the late Fred Hirshfeld said, "An accurate set of nuclear coordinates and a detailed map of the electron density can be obtained, by X-ray diffraction, only jointly and simultaneously, never separately or independently."

The book contains 12 chapters in a logical order from the fundamentals to applications to specific types of systems in the final three chapters, i.e., transition metal compounds, extended solids, and molecular crystals. The first chapter goes into the theory of scattering of X-rays and neutrons. The second chapter discusses the important topic of the effect of thermal vibrations on the intensities of the diffracted beams including anharmonic effects. In the third chapter the relationship between the chemical bonding and the scattering formalism is presented. The breakdown noted above in the independent-

atom model for the electron density (i.e., superposition of spherical atoms) is explored, and the improved scattering models needed are given. Included are multipolar methods and the κ refinements.

In chapters four and five least-squares and Fourier methods are given as well as the recent technique of maximum entropy enhancement. However, little mention is made of the latest developments in density matrix refinements. The next three chapters contain methods for spatial partitioning and topological analysis of the charge density as well as the electrostatic moments and electrostatic potential. In Chapter 9 the role of the charge density in the cohesive energy of crystals is examined.

The author has been very careful in the presentation of the material. For example, he cautions the reader in presenting the Gram-Charlier expansion that the Hermite polynomials employed are not those familiar from the quantum mechanical treatment of the harmonic oscillator. The latter involve the n th-order derivative of $\exp(-x^2)$; the former, used mostly in statistics, involve the n th-order derivative of $\exp(-1/2x^2)$ and are sometimes given the symbol $He_n(x)$ to avoid confusion with the latter, denoted by $H_n(x)$.

Many concepts from quantum chemistry including density functional theory are introduced and used in the book. However, I would suggest that in the next edition an appendix be added in which some of the language and methods of modern computational chemistry are mentioned. This would include basis set nomenclature and quality descriptors. Another useful appendix would provide information about the needed computer programs and their sources.

As expected there are some typographical errors which do not detract from one's progress through the book. Gremlins have left their tracks in eq 1.50 and Figures 11.10, L.1, and L.2. The caption of Figure 1.7 is confusing because this figure is a plot of f' vs f'' . One thing that I like to check is how a book treats a fundamental theorem in Hartree-Fock theory. In one line on p 186, it is called Koopman's theorem; two lines later it is correctly named Koopmans' theorem.

This book is a worthy member of the series of books sponsored by the International Union of Crystallography (IUCr). It opens up this area to a wider audience. Not only is it valuable to the specialist as a reference but it can help refresh one's mind on the technical aspects of the subject.

Vedene H. Smith, Jr., *Queen's University*

JA975636D

S0002-7863(97)05636-9

Progress in the Chemistry of Organic Natural Products, #71. Edited by W. Herz (Florida State University), G. W. Kirby (University of Glasgow), R. E. Moore (University of Hawaii), W. Steglich (Universität München), and Ch. Tamm (Universität Basel). Springer: Wein, Germany. 1997. \$219.00. ix + 358 pp. ISBN 3-211-82850-8.

This is the current volume of a long-standing series on the chemistry of organic natural products. This volume masterfully maintains the tradition of the series by presenting its subject matter in a clear, organized, thorough, and visually appealing style. There are three chapters of varying lengths on insect neuropeptides by G. Gäde, sesquiterpenes from *Thapsia* species by S. B. Christensen, A. Andersen, and U. W. Smitt, and pregnane glycosides by D. Deepak, S. Srivastav, and A. Khare. Each review is thorough, accurate, and carefully referenced, covering isolation, structure elucidation, and biological activity. References are current through 1995, and there are detailed subject and author indices. This book will be an essential addition to the bookshelves of all chemical libraries, and will be an invaluable reference source for workers interested in natural products chemistry.

Robert S. Coleman, *The Ohio State University*

JA9756836

S0002-7863(97)05683-7