Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

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X-ray charge densities and chemical bonding. By PHILIP COPPENS. Pp. xiii + 358. Oxford: International Union of Crystallography/Oxford University Press, 1997. Price US $85.00. ISBN 0-19-509823-4.

The extraction of the detailed distribution of electrons in solids from X-ray diffraction data used to be a kind of 'luxury passion' indulged in only by a few 'gourmet' crystallographers, theoreticians and experimentalists who could afford to face its difficulties and dare to confront its often limited success. This activity has passed beyond that stage and established itself as a comprehensive experimental method for gaining genuine and mostly unique chemical information on atomic and molecular systems in the crystalline state. Owing to recent advances, it is becoming a readily affordable and an almost routinely executable technique. Nevertheless, there has been no proper textbook available to summarize the basic aspects of the field for a broad community – a weighty reason to welcome the title volume whose author needs no introduction. His name tells us as much about the topic of the book as does the title. Professor Coppens has pioneered the development of the method and his research has highlighted all the major steps in its evolution to a discipline.

The aim of the book, the fourth in the series of *IUCr Texts on Crystallography*, is 'to provide the background necessary for interpretation of the results of accurate crystallographic methods and to present the concepts to a wider community of nonspecialized scientists' – a well formulated goal hinting at the interdisciplinary nature of the topic. Although the text is not meant as a review, the basic principles are illustrated, unavoidably without completeness, by examination of relevant studies from the last decades.

The volume is divided into twelve chapters supplemented by Appendices covering the necessary mathematical formalisms. The introductory paragraphs outlining the chapters are its first appealing feature. The leading chapter is devoted to an introduction to the theory of scattering and provides the reader with details of both the classical and quantum-mechanical descriptions of the relevant phenomena. By use of the Fourier convolution theorem, the complicated subject is covered smoothly and elegantly. That topic is followed by an inclusive treatment of the effect of thermal motion on diffracted intensities. This chapter is rather didactic than rigorous, but it cites the important theoretical texts needed to fill in the details. It includes formalisms beyond the usual harmonic approximation and gives an introduction to the statistical approaches as well as to the kinematic model of rigid-body motion. The next chapter deals with advanced X-ray scattering formalisms accounting for chemical bonding. It starts with qualitative considerations of the structural evidence that indicates the limitations of the conventional model, then discusses the modified spherical-atom scattering formalism. The multipolar expansion, the most popular and successful technique used at the forefront of research and applications, is outlined and its connection with the LCAO description of the electron density is demonstrated. The parameters of the density model are derived by fitting the predicted structure factors to those measured. The procedure is based on the method of least squares, which is discussed in subsequent paragraphs. The reader is then guided to details of alternative and competing approaches, such as the Fourier method and maximum-entropy enhancement. The analysis of the electron density requires space partitioning, different methods of which are described in ch. 6. Bader's theory of atoms in molecules attributes a paramount importance to the charge distribution, from the topology of which one may derive all static and reactive properties of an electronic system. It is shown here how the interpretation of experimental densities benefits from modern quantum theory. The next three chapters give an exciting account of how to extract density-related physical properties from diffraction data. The electrostatic moments, potential, field, field gradient and lattice energy are considered with a high level of mathematical rigor. The remaining parts provide the reader with a wide variety of chemical applications: charge-density studies on transition-metal complexes, excited solids and molecular crystals, these last having been the major objective of the research because of their suitability for experimental analysis.

The twelve Appendices cover a considerable part of the mathematical details, though these are already treated, to some extent, in *International Tables for X-ray Crystallography*. A reader keen to develop some practical knowledge will enjoy the interesting and useful exercises put forward at the end. The references are well grouped and the index offers a clear navigation through the book. If the book has a deficiency, it lies in its complete neglect of experimental methods, most probably a deliberate choice on the author's part given their rapid ongoing and not yet conclusive development.

Professor Coppens's book improves our basic understanding of the subject, and its didactic aspect should be emphasized when comparing it to the related text by V. G. Tsirelson & R. P. Ozerov (*Electron density and bonding in crystals*, Institute of Physics Publishing, 1996), which is a less balanced monograph in the sense of offering more to the specialized than to the novice reader. The author is to be congratulated for producing this impressive volume which is a coherent text, meeting its goals in all respects, which will be appreciated by all scientists with an interest in the fine details of molecular structure.

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