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BOOK REVIEWS

X-RAY DIFFRACTION AND THE IDENTIFICATION AND ANALYSIS OF CLAY MINERALS, 2nd Edition. By D. M. Moore and R. C. Reynolds Jr. Oxford, New York, 1997. 378 p. $36.00

Reading the second edition of Moore and Reynolds' *X-ray Diffraction and the Identification and Analysis of Clay Minerals* is an absolute delight. It is rare to come away from reading a scientific book with a feeling of excitement and motivation. However, I was consumed by the infectious enthusiasm of the authors as a result of their dynamic, personable, and clear writing as well as their frequent use of humor. The second edition has retained the excellent parts of the first edition, revised several important sections of the first edition, and added an enormous amount of new, relevant information particularly in the areas of importance of clay minerals, physical properties of clay minerals, clay petrology, and X-ray diffraction of mixed-layered clay minerals. By increasing the number of lines per page, increasing by 15% the total number of pages, reducing font size in the reference list, and decreasing figure size (without sacrificing clarity), the second edition includes 50% more text and double the number of references (which now total over 500) compared to the first edition. The improvements have broadened the scope of the book significantly.

Chapter 1 introduces the subject of clay mineralogy and provides a fascinating history of the serendipitous discovery of X-rays by Röntgen and the discovery of X-ray diffraction (XRD) by von Laue. The chapter ends with the history, importance, and literature of clay mineralogy. A significant improvement over the first edition is the section on the importance of clay mineralogy, including a discussion of clay minerals as catalysts and the expanded list of references, which includes many helpful annotations. Chapter 2 covers the nature and production of X-rays, including both theory and methodology. This chapter contains new sections on "other" analytical techniques for studying clay minerals and the definition of radiation dose. Although the authors continue to use older, manually operated X-ray diffractometers as their preferred method for teaching the operations of a diffractometer, they include an important new section about step scanning with a computer-automated diffractometer. This section contains valuable practical advice on how to generate high quality XRD data. Chapter 3 covers X-ray diffraction including X-ray scattering, constructive and destructive interference, Bragg's law, and the mathematics of diffraction from crystals. There is an exercise on calculating peak intensity for the (001) *d*-spacing of illite and a new section on the reciprocal lattice.

Chapter 4 covers general structures and physical properties of clay minerals with new coverage of octahedral vacancy and kaolin polytypes. However, the greatest improvements to this chapter are in the discussion of physical properties of clay minerals, which includes coverage of permanent and variable (pH-dependent) charge on clay minerals, the electrical double layer, flocculation, cation exchange, swelling, and clay-organic interactions (complete with an introduction to the terminology of organic compounds). I think, however, that this discussion of physical properties of clay minerals would work better if it were placed after Chapter 5, which covers the structures of individual clay minerals. As it stands, Chapter 5 describes the structure, composition, and occurrence of individual clay minerals in much greater detail than the first edition. More clay minerals are covered, particularly for minerals in the serpentine, vermiculite, and mixed-layered clay groups. A much greater depth of coverage exists for all clay mineral groups. There are new and interesting sections on industrial uses of kaolin and the formation of bentonite and tonstein. Chapter 5 also provides a considerable updating of recent work on the smectite-to-illite reaction. Finally, there are excellent exercises on calculating structural formulas and constructing structural models of layer silicates.

Chapter 6 continues to be an outstanding treatment of sample preparation techniques of clay minerals for XRD analysis. There is a new section on freeze-drying procedures for analysis of randomly oriented powders. Chapter 7 describes XRD identification of clay minerals and associated minerals. The inclusion of calculated XRD patterns instead of tables of *d*-spacings and intensities is particularly effective as an instructional method. There is a new section on calculated XRD patterns of disordered silica minerals (cristobalite and tridymite). A substantially revised Chapter 8 covers XRD identification of mixed-layer clay minerals. New material includes examples of the use of peak broadening to characterize mixed-layered clay minerals, the effect of poor-quality, noisy XRD data on interpretations, and of XRD identification of mixed-layered kaolinite/smectite and other mineral mixtures, including mixed-layered clays plus non-interstratified clay minerals. Chapter 9 summarizes well the theory and practice of quantitative mineral analysis by XRD, including the methods of external standards and of orienting internal standards. All new Chapter 10 describes XRD methods for characterizing 3-dimensional stacking disorder in smectite, mixed-layered illite/smectite, and illite. The chapter discusses composite XRD patterns that illustrate the procedures for characterizing different kinds of disorder (turbostratic stacking, rotational disorder, and octahedral vacancy-induced disorder). The book ends with an appendix that summarizes the NEWMOD computer program used to calculate one-dimensional XRD patterns for clay minerals.

The book succeeds in being a combination textbook and lab manual for clay mineralogy students and researchers in the fields of geology, soil science, engineering, and chemistry. The

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paperbook and ring binder format (which allows the book to lie flat on a lab bench) as well as relatively low cost are all real advantages. The second edition of this book belongs on the shelf of every student, teacher, and researcher in the field of clay mineralogy, regardless of whether you own the first edition.

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X-RAY CHARGE DENSITIES AND CHEMICAL BONDING. By P. Coppens. Oxford University Press, 1997. 358 p. $85.00

When the results of experimental electron density studies are presented to non-specialists, these results are sometimes viewed with skepticism simply because there is insufficient time to relate the details of the methods used. This book is truly a textbook on the methods of experimental electron density analysis. It is intended for the non-specialist. The author has been an internationally recognized leader in the field for over 30 years. His deep understanding of the field is reflected in how easily he guides the reader through what appear to be treacherous shoals. The book is superbly written.

Chapter 1 covers X-ray and neutron diffraction in the first Born approximation. The effects of both harmonic and anharmonic vibrational motion on Bragg intensities are covered in Chapter 2. In traditional X-ray structure analysis the electron density of the crystal is assumed to be a superposition of neutral, spherical atoms. In Chapter 3 it is shown how this approximation leads to errors and how the electron density model of the crystal can be modified to better fit the measured X-ray data by allowing the atoms to deform in a general way; the so-called multipole formalism. Chapter 4 covers the basics of the least-squares method as applied to charge density analysis. Much of the early charge density work relied on Fourier difference maps to resolve bonding electron density. Fourier methods are covered in Chapter 5. Chapter 5 also covers the recently introduced maxiumum entropy enhancement of experimental charge densities.

By the end of Chapter 5 the reader will have a good understanding of how detailed electron density distributions are retrieved from accurate X-ray diffraction data. Chapters 6 through 9 are largely devoted to showing what can be learned from these distributions once they are obtained. In Chapter 6, various methods of partitioning both the deformation and total electron densities are introduced. In addition, the topology of the total electron density is discussed, including the relationship between the Laplacian of the electron density and chemical bonding. Chapter 7 explains how molecular dipole, quadrupole, and higher order electrostatic moments may be obtained from X-ray diffraction data. Chapter 8 shows how the electrostatic potential, electric field, and electric field gradient may be mapped. The electrostatic potential is the most accessible electrostatic property that can be obtained from mineral X-ray data as long as extinction is kept to a minimum. In Chapter 9, the author shows, via density functional theory, how the cohesive energies of both ionic and molecular crystals may be obtained once an accurate electron density distribution has been retrieved from X-ray measurements. Finally, Chapters 10 through 12 review work completed on transition metal compounds, extended solids (including silicates), and molecular crystals. An extensive set of references accompanies each chapter in the text. In all of the chapters where various methods and properties are discussed, specific examples are shown either from the work of the author or from other leaders in the field.

For those planning to work in the field, extensive appendices provide much useful information. For example, an entire appendix is devoted to symmetry restrictions on temperature factor tensors, another on probability ellipsoids. For use in the multipole formalism, four appendices are devoted to spherical harmonic functions and their products, exponents for single-ζ wavefunctions, and Fourier-Bessel transforms of Slater-type radial functions. Also included is a short set of exercises that covers most chapters of the text. This comprehensive text on experimental electron density analysis is a must for any serious practitioner in X-ray crystallography. For students, this book will provide a more in-depth review of X-ray diffraction than is found in modern texts, which have become more and more non-rigorous in their treatment. For those doing conventional X-ray structure analysis, this book will reveal that there is more to be obtained from X-ray diffraction data than atomic positions and vibrational parameters.

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