

Structural classification of minerals.

Vol. 1. By J. Lima-de-Faria. Dordrecht: Kluwer Academic Publishers, 2001. Pp. xi + 143. Price EUR 54.00, US\$ 58.00. ISBN 0-7923-6892-4.

Over the centuries there have been many attempts to find effective ways of classifying the natural objects found in the world around us. Linnaeus discovered the way to classify plants in the eighteenth century but the classification of minerals has proved more elusive. Early schemes classified them according to their uses (gems, ores). Later schemes were based on physical properties (hardness, colour), chemistry (carbonates, silicates) or crystallography (symmetry, interfacial angles). It was not until the work of Bragg and his contemporaries in the first half of the twentieth century that it became possible to see how the internal structure of crystalline minerals provided the link between these different schemes and helped to explain the anomalies. The different habits of fibrous and sheet silicates, for example, were seen to be a direct consequence of the ways in which the silicate tetrahedra are linked within the crystal.

Recent attempts to classify minerals, such as Liebau's work on the silicates and Hawthorne's hierarchical principle, are based on the topology of the bonds that link the atoms in the crystal. Lima-de-Faria, who has spent much of his career in developing a comprehensive structure-based classification of minerals, follows this route in the projected three-volume series *The Structural Classification of Minerals*, of which the volume under review is the first, dealing with elemental, binary and ternary minerals.

There is no doubt that the best approach to mineral classification is one based on the structure at the atomic level. This structure is determined by the ability of the constituent atoms to express their ideal coordination numbers and bond lengths in three-dimensional space, while at the same time adopting the energetically favoured highest possible symmetry and most compact packing. This collection of constraints is formidable and explains why both chemistry and symmetry are important elements in the understanding of mineral structure. The physical properties, and ultimately the uses

book reviews

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to which the minerals are put, follow from this structure.

The structure of a mineral is best described in terms of the sites occupied by the elements present. A given atomic site in the crystal may provide a suitable location for several different chemical elements, and, if all these elements were present in the melt from which the mineral was crystallized, they may all be found at this same site in the crystal. The proper description of such a solid is not one based on the chemical composition, but one based on the occupation of different atomic sites. This is reflected in the difference between the chemical and structural formula. A chemical formula consists of a list of element symbols, each followed by its multiplier. A structural formula, on the other hand, consists of a list of atomic sites, each atomic site being represented by the symbols of all the elements that occupy that site. For example, a compound that has the chemical formula CoMgSiO_4 might have the structural formula $(\text{Co}_{0.8}\text{Mg}_{0.2})(\text{Mg}_{0.8}\text{Co}_{0.2})\text{SiO}_4$, indicating that the Co and Mg atoms are disordered over two crystallographically distinct sites. In spite of their similar appearance, the two types of formula express fundamentally different information, a distinction that is important for the classification of minerals (and other inorganic compounds). Lima-de-Faria, following the recommendations of the IUCr Commission on Crystallographic Nomenclature, introduces a more elaborate version of the structural formula in which additional symbols indicate the coordination environment of each site and the relationships between them. These elaborated structural formulae form the basis of the classification used in this book. Even so, it is possible to classify some minerals in more than one way. Some might be surprised to find forsterite, Mg_2SiO_4 , classified as a close-packed structure rather than as a complex, though this is logical given its relationship to the close-packed structure of spinel, MgAl_2O_4 .

Volume 1 is a comprehensive listing of around 1000 elemental, binary and ternary minerals. Volume 2 will contain all the other anhydrous minerals and Volume 3 will cover the hydrated minerals. Although Volume 1 contains a brief review of the author's

system, the reader will need to consult his earlier work: *Structural Mineralogy. An Introduction*. [Lima-de-Faria, J. (1994). Dordrecht: Kluwer Academic Publishing] in order to fully appreciate the nature of the classification. For example, an important set of tables in Volume 1 illustrates the structure types using the author's 'condensed models' (diagrams) but there is no description of how they are constructed or how they are used. Unfortunately, their interpretation is not intuitive. They consist of rafts of overlapping circles representing layers of close-packed atoms and the cavities between them. Some circles are large, some small, some are filled and some are empty, but there is no explanation of the conventions used. In order to understand these diagrams the reader must consult the earlier volume. This may not be a serious problem since anyone buying the present book will probably already own a copy of the earlier work which, apart from describing the system of classification in detail, gives a classification of the 300 most common minerals.

After a brief ten-page introduction to the method of classification, the remaining 112 pages are devoted to three sets of tables. The first set, comprising Tables 1–72, gives a comprehensive listing of all the minerals that fall within the scope of the work. The tables are arranged by their chemical formula class (A, AB, AB_2 etc.). Within each table, the minerals are arranged alphabetically by name. A considerable amount of information is given for each mineral – its structural formula, space group, unit cell, the Wyckoff positions of its atomic sites, its structure type (as defined by the archetypal mineral) and references (mostly to standard compilations such as Wyckoff). The second set of tables, comprising Tables 1L–17L, describes 52 structure types using the author's condensed models, described above, and the third set, comprising Tables 1S–26S, is a listing of the minerals by structure type, arranged first by chemical formula class and then by structure class (close-packed, complex, chain, layer, framework). The book ends with a list of abbreviations, an alphabetical index of minerals, a very short (34 items) subject index and a slightly longer author index. This arrangement allows a mineral to be readily located by name, by structure type,

or by chemical class. The tables are well laid out and, subject to the above reservations about the condensed models, they are easy to use.

The listing contains only minerals, *i.e.* natural materials recovered from the earth, but with this restriction the listing is comprehensive. The book should therefore be of considerable interest to mineralogists. However, classifying minerals according to their internal structure is somewhat akin to classifying mineralogists according to their internal structure. Both are valid exercises, but in both cases the objects classified represent but a small sample arbitrarily selected from a much larger population of objects with similar internal structures. One is left with the feeling that the same classification could usefully be extended to their non-mineralogical brethren and that the properties of minerals (or mineralogists) would be better understood if placed in this larger context. The book does serve to illustrate the differences between the approach of the mineralogist and the approaches of other solid state scientists. For example, in this book the orthorhombic mineral perovskite, CaTiO_3 , (the space group given curiously as *Pcmn*) is taken as the archetype of the seven minerals that have this, or a closely related, structure. This choice will seem strange to a condensed matter chemist or physicist who would describe the structure type by its aristotype, a crystal such as tausonite, SrTiO_3 , which has the high symmetry cubic *Fm $\bar{3}$ m* structure. Such people will likely be frustrated by the absence of any synthetic crystals in this listing, though they may be interested to see where the familiar names of the structure types come from. In fairness, the author does not pretend to address the needs of this group, and including even a small fraction of the important synthetic compounds would

have produced a much larger work which would have compromised the elegance of the presentation.

This book is essentially a catalogue of simple minerals organized on the rational basis of structure. In this it is successful and likely to be of value to anyone interested in understanding the similarities and differences in the chemical and physical properties of minerals.

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books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Chirality: physical chemistry. Edited by Janice M. Hicks. (ACS Symposium Series, #810). Pp. ix + 356. New York: Oxford University Press, 2002. Price US\$ 140.00. ISBN 0 8412 3737 9. This book 'evolved from the first symposium on the Physical Chemistry of Chirality held in San Francisco, California at the National Meeting of the American Chemical Society . . . in March 2000'. The editor's intention is 'that those studying interesting new chiral systems will interact with those at the forefront of developing new methods for

studying chirality both experimentally and theoretically, in order to stimulate new research directions'. Two of the 22 contributions report on the new phenomenon of X-ray natural circular dichroism (XNCD).

Physics of ice. By Victor F. Petrenko and Robert W. Whitworth. Pp. xiii + 373. New York: Oxford University Press, 2002. Price US\$ 65.00 (paper). ISBN 0 19 851894 3. A paperback reprint of the book of the same title published in 1999. The 13 chapters in this excellent book cover all aspects of the physical properties of ice in its various manifestations and serve to remind us of the complexity of this material and its importance. Emphasis is placed on the relationship between crystalline structure and the properties of the water molecule. A penultimate chapter, of general interest, *Ice in nature*, offers a wealth of observations on ice on and in land, sea, air and the solar system. A useful bibliography and 43 pages of references underline the widespread study ice attracts.

Physics meets mineralogy: condensed matter physics in the geosciences. Edited by H. Aoki, Y. Syono & R. J. Hemley. Pp. xi + 397. Cambridge University Press, 2000. Price £65.00, US \$100.00. ISBN 0-521-64342-2. A review of this book, by Georg Amthauer, has been published in the May issue of *Acta Cryst.* Section A, page 303.