

BOOK REVIEWS

BUERGER (MARTIN J.). *Vector Space and its application in crystal structure investigation*. New York (John Wiley and Sons) and London (Chapman and Hall), 1957. 347 pp. Price \$12 or £4. 16s.

This book describes the application of the Patterson Function to X-ray crystal structure analysis.

The starting-point in crystal structure analysis is the set of experimentally determined intensities, $|F(hkl)|^2$, associated with the diffraction pattern of the crystal. The difficulty is that of determining the phases of the reflections. A. L. Patterson showed that the experimentally determined $|F(hkl)|^2$ used as coefficients in a Fourier synthesis give maxima that represent the lengths and orientations of the interatomic and intermolecular vectors *but not the positions of the atoms* in the crystal.

Although this is theoretically possible, the Patterson Function is difficult to interpret because maxima may represent the superposition of several vectors, and often Patterson maps display a uniformity of peak heights particularly if the crystal unit cell contains many atoms of about equal scattering power, for example carbon, nitrogen, and oxygen in organic compounds. In most cases where the Patterson Function has been successfully applied, the crystal contains atoms either of widely differing X-ray scattering power, or the atoms have some peculiar stereochemical configuration as in conjugated ring systems.

In spite of this difficulty of interpretation, the Patterson Function contains all the available diffraction information about the crystal. Since the war, there have been many attempts to put the direct interpretation of this function on to a quantitative basis. Having himself made significant contributions in this field, Professor Buerger shows authoritatively how this may be done in principle and practice. The Patterson Function is widely used in crystal structure analysis but is bewildering to a beginner; Professor Buerger is to be complimented on his attempt to treat it as a subject in itself.

The book may roughly be divided into two parts. The first nine chapters deal with the early use and the theory of the Patterson Function. Here Buerger has shown the relationship of Patterson symmetry to crystal symmetry and in these chapters one sees the experience of a good teacher taking the beginner over the many pitfalls of this subject. The next four chapters deal with image-seeking functions and superposition methods, which form the basis of the interpretation of Patterson

Functions. The book is well illustrated with examples of the determination of structures involving these techniques; quite a few have been worked out in Buerger's own laboratory, but as mentioned earlier all these examples depend for their solution either on the presence of heavy atoms or some known geometrical configuration of the components of the unit cell. There is a very useful list of references at the end of each chapter to published work in X-ray crystal structure determinations using these methods.

The book is singularly free of major errors. Nevertheless it has two main shortcomings. The first is that it is too bulky for a treatment of one particular aspect of crystal structure determination and the author could well have presented the same arguments in half the number of pages, thereby reducing the price of the book and so bringing it into the hands of more beginners, for whom he must have intended it. The second criticism is the author's failure to warn the beginner both of the limitation and of the difficulties of the interpretation of Patterson vector maps. A minor criticism is the insufficient mention of the increasing and important use of 'sharpened' Patterson Functions in the structure determination of complex compounds, as for instance vitamin B₁₂.

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BURRI (Conrad). *Petrochemische Berechnungsmethoden auf Äquivalenter Grundlage (Methoden von Paul Niggli)*. Basel and Stuttgart (Birkhäuser Verlag), 1959, 334 pp., 66 text-figs. Price (bound) 38 Swiss fr.

The late Professor Paul Niggli introduced several methods for handling chemical analyses of rocks both to use them as a basis for classification and to calculate their actual or potential mineral composition. These methods are scattered through Niggli's many publications. The author here has collected them together and, by means of fully worked out examples, he explains the methods and illustrates their uses. No one is better qualified to do this than the author, who worked very closely with Niggli for many years at Zürich where he is Professor of Petrography.

An introduction reviews the various methods of graphical and diagrammatic presentation including triangular and tetrahedral diagrams. The first main chapter, 100 pages, deals with 'Niggli values' and their calculation from and to wt. %, cation %, and mol. (equivalent) %. The calculation of silica saturation (the 'quartz number'), norms and normative feldspars, and other values (*k*, *mg*, &c.) are explained. A projection of the *al-fm-c-alk* tetrahedra is used to depict eruptive fields,