

suffered slight dehydration, while the new specimen possibly contains a little unbound water or CO_2 .

Comparison of observed and calculated specific gravities supports the new formula $3\text{CaO}\cdot 6\text{SiO}_2\cdot 8\text{H}_2\text{O}$. Eakle reported a specific gravity of 2.206. We have made new determinations, by the suspension method, and find 2.24 ± 0.01 for the type specimen and 2.23 ± 0.01 for the new specimen. The values calculated for either specimen from the cell dimensions are 2.14 for the old formula and 2.26 for the new formula. Heller and Taylor (1956) quote a calculated value of 2.28 for the old formula, but this is wrong.

We are studying the crystal structure and the products and mechanism of dehydration. We thank the U.S. National Museum for the loan of the type specimen (USNM 95637), and Dr. A. B. Carpenter of Harvard University for a generous portion of the new specimen (Com 203).

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GARD (J. A.) and TAYLOR (H. F. W.), 1956. Min. Mag., vol. 31, p. 5.
HELLER (L.) and TAYLOR (H. F. W.), 1956. Crystallographic Data for the Calcium Silicates. H.M.S.O., London.

BOOK REVIEW

WOOLFSON (M. M.). *Direct Methods in Crystallography*. Oxford (Clarendon Press—Monographs on the Physics and Chemistry of Materials), 1961, 144 pp. Price 30s.

To determine the arrangement of atoms within the unit cell of a crystal one requires to find a set of structure factors F_{hkl} , one for each order of diffraction (hkl); from these, a map showing the atom positions can readily be calculated. In general F_{hkl} is a complex quantity, and one can only measure F_{hkl}^2 from the intensity of the hkl diffracted X-ray beam; the phase angle for each F_{hkl} remains to be determined. The problem is much simplified if the crystal structure (or that projection of it that is being examined) has a centre of symmetry, when all phase angles are 0° or 180° ; in this case one has only to decide whether to take the positive or the negative square root of F_{hkl}^2 . Even so there are too many structure factors involved for direct guesswork.

Most crystal structures have been determined starting from an approximate idea of the location of at least some of the atoms. Structure factors are calculated from those locations assumed and the observed F_{hkl} are used with the calculated signs to obtain a map from which more exact locations can be obtained and at least some of the previously unlocated atoms can be placed. These results are used to calculate new structure factors and the new signs used for a new map, and so on, until for a map the assumed and derived locations for all atoms agree. Thus the problem is to obtain sufficient clues as to the structure to start this process, avoiding false assumptions that fail to refine neatly in the manner described.

Data about the structure can be derived intuitively from the unit cell dimensions, the known size and chemical bonding of the atoms to be located, and the physical properties of the crystal. More rigorously, the known values of F_{hkl}^2 can be used without knowledge of signs to form a so-called Patterson map which shows, not the positions of the n atoms in the unit cell, but those of the $\frac{1}{2}n(n-1)$ vectors between pairs of atoms. Provided n is not too large, methods are available for interpreting Patterson maps in terms of atomic positions; very often, even if n is relatively large, the positions of a few heavy atoms, if present, can be found and a start can thus be made on the refinement.

During the last decade, more direct methods have been developed for determining the *probable* signs of structure factors for centrosymmetrical structures (and projections). These do not involve any assumptions about atomic positions, but consider only the magnitudes of the structure factors themselves. Several practicable methods, suitable for larger or smaller values of n , have now been developed and proved successful. These methods appear to work best for structures containing only fairly equal atoms, and thus complement the Patterson approach.

A review of direct sign-determining methods is by now appropriate and is given in this book in an entirely admirable way. The approach is severely practical; detailed derivations of formulae are relegated to appendices and the text is developed in relation to fully worked examples; further examples, with solutions, are left as exercises for the reader. The author's style is stimulating and highly readable, and your reviewer, previously unacquainted with these developments, can at least testify to feelings of confidence, even eagerness, at the prospect of at least embarking on an application of direct methods to a structural problem. Both the author and the publishers are to be congratulated.

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