

There are three brief appendices on computing transforms and on obtaining them by optical methods, with the handsome plates one has come to expect from the authors. The reviewer only wishes that a good deal more of their beautiful published work (including plates) had found its way into their book.

Highly useful features are a system of numbering equations which includes the page number on which a given equation appears, and indication in the reference list of the pages to which any given reference applies.

In summary, this is a handsome, if too brief, monograph which will be of interest to anyone doing structural work.

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### References

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 HOPPE, W., LENNÉ, H. V. & MORANDI, G. (1956).  
*Z. Kristallogr.* **108**, 321, and later papers in *Z. Kristallogr.*  
 WASER, J. & SCHOMAKER, V. (1953). *Rev. Mod. Phys.* **25**,  
 671.

ТЕОРИЯ СТРУКТУРНОГО АНАЛИЗА. By  
 А. И. КИТАЙГОРОДСКИЙ. АНАЛИЗА ИЗДАТЕЛЬСТВО  
 АКАДЕМИИ НАУК СССР. Москва - 1957.

**The Theory of Structural Analysis.** By A. I.  
 КИТАЙГОРОДСКИЙ. Publishing House of the Academy  
 of Sciences of the USSR. Moscow. 1957. 283 pages.  
 Price 10 rubles, 65 kopeks.

This concentrated book sets forth the methods which can be used to find the atomic arrangement in a crystal, after the diffraction data—X-ray, electron, or neutron—have been collected and reduced to tables of the magnitudes of the structure factors  $|F(hkl)|$ .

The first chapter contains a mathematical introduction concerned mainly with Fourier transforms, convolutions of functions, and the concept of reciprocal space. The second chapter presents a neat and condensed development of kinematic theory of the scattering of radiation by objects, both amorphous and crystalline, and defines the structure amplitudes,  $F(hkl) = F_H$ , and the 'structure products',  $F_H F_K F_{H+K}$ , etc., to which the author has devoted so much fruitful and original work.

Chapter III is devoted to the statistical properties of structure amplitudes and products. The work of A. J. C. Wilson and his colleagues is presented and developed by the author to apply to structure products. The notion of 'unitary' structure factors is extensively used here, as well as elsewhere throughout the book (to the delight of this reviewer). The identification of symmetry elements by statistical methods is well described, and the predominant positivity of the structure product  $F_H F_K F_{H+K}$  is derived in what is believed to be a new and illuminating way.

Chapter IV is a very complete exposition of inequality methods for establishing the signs of structure amplitudes and products. In it is a great deal of original development by the author, who states that his direct methods are successfully applicable to all cases where other methods work. A defect in this chapter, it seems to this

reviewer, is the lack of a presentation of the valuable work of Karle & Hauptman; these authors are merely mentioned as having developed methods of sign determination which also work. Another omission is any discussion of the problems in phase determination presented by crystals without centers of symmetry; this reviewer feels strongly that the structures of crystals such as these will be important subjects of research during the coming years.

Chapter V, entitled 'A Study of the Convolutions of the Electron Density', contains a treatment of the Patterson function. This treatment is quite mathematical—not one example of a Patterson function is depicted—but contains the essentials of the methods being used at present in solving crystal structures. The author refers the reader who wishes to know more about the practical use of the Patterson method in structure determination to the published work of others.

Chapter VI—the last one—is concerned with methods of refining structures. Sections are devoted to the  $R$ -factor, Booth's method of steepest descent, least squares, the differential method, and the difference method. The estimation of the error of a structure determination is the subject of an original treatment, toward the end of which appears the comment: 'We see that a deterioration in the accuracy of the determination of the structure amplitudes to 50% (this means 100% for the intensities) has little effect on the result of the analysis'. This refers, of course, to atomic positions; but even for these—in the opinion of this reviewer—precise bond distances and angles cannot be obtained from such data, and the discovery of atomic shapes and ionizations, bonding effects, hydrogen positions, etc., is quite impossible under these conditions.

The book ends with a three page 'Conclusion' which states, in essence, that structures containing more than about 100 atoms per asymmetric unit are impossible to solve by diffraction methods. This is probably true if one is limited to the methods described in this book—methods which make use of only one crystalline specimen. This reviewer feels he must point out that other methods are known, such as the isomorphous replacement method, or the use of anomalous dispersion, which can be extended to much more complicated structures, and also that the history of the subject shows that new methods are discovered from time to time which progressively increase the complexity of the structures capable of solution. As a counterbalance to the pessimistic flavor of his last statement, the author points out that the determination of crystal structures is now ready, in principle, to be made fully automatic—computing machines could be programmed to work directly on the observed intensities and come out with the atomic positions in crystals having up to perhaps 20 atoms per asymmetric unit.

This is a good book and contains much of the author's original work on the subject. Every X-ray crystallographer could benefit from a study of this volume. It is another one in the growing number of reasons why every professional scientist should acquire at least a reading knowledge of the Russian language. Meanwhile a translation of the book is due to appear shortly (Consultants Bureau, Inc., New York, Publishers).

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