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Editorial Preface

Crystallography was transformed into an effectively new science by the discovery of X-ray diffraction in crystals in 1912 In the following two decades, an enormous development took place, forging into a practical tool what had originally been a physical experiment, and the atomic structures of hundreds of substances of ever-increasing complexity were established. No second spectacular crystallographic discovery has since been made of consequences comparable with those of the original discovery of X-ray diffraction, but general progress in methods has been such as to result in opening up many new possibilities for research in the immediate future. The following are examples of major developments:

(1) The exploitation of Fourier methods for general structure analysis and for the study of chemical bonds. Allied with this development, calculating machines and optical methods for dealing with the Fourier analysis and Fourier synthesis of complex molecules have been devised.

(2) The general progress in the classification and calculation of inter- and intramolecular forces.

(3) The investigation of some co-operative phenomena, such as order-disorder in alloys, the transition of ferro-electrics at the Curie points, and the incidence of rotation of atomic groups in some crystals.

(4) The relation of mechanical and magnetic hardness in crystalline material to periodic modulations of the crystal structure.

(5) The construction of powerful X-ray tubes and the perfection of monochromators, permitting the observation of low-angle diffraction effects.

(6) The discovery of diffuse X-ray reflexions associated with thermal motion, and of their importance for the study of the atomic forces within the crystal.

(7) The study of partially crystalline substances, such as rubber, plastics, fibres and other high polymers.

(8) The extension of X-ray analysis to the extremely complex molecules of protein viruses and other biological substances.

(9) The development of a micro-analytical technique of X-ray analysis for establishing the chemistry of substances obtainable only in fractions of a milligram, such as plutonium in the pre-pile days.

(10) The perfection of electron microscopy to the stage of providing a direct image of the regular array of molecules in certain cases.

In addition to these purely scientific advances crystallography has penetrated further than ever before into the technical processes of various industries; the chemical, ceramic, metallurgical, optical and radio industries are obvious examples. The problems there arising often suggest an interesting starting point for a more comprehensive academic research, as, for example, in the case of the method recently described for the untwinning of quartz.

This journal is therefore starting at a time of great promise for interesting new developments in crystallography. Wide fields of future research are opening up. Much is yet to be learned about the general mechanism of crystallization, including the reasons for the transitions of a substance from one crystalline form to another; about the mechanical, electrical, optical and plastic properties of crystals in relation to atomic forces and structure; about the internal perfection and imperfection of crystals and the consequences thereof; about chemical bonds, surface forces, diffusion and chemical reactions within the solid; about the diffraction of atoms, electrons, neutrons and, possibly, of other particles by crystals. Many problems arise from the study of substances which show a periodicity less perfect than the three-dimensional one of true crystals. Fibres, high polymers, and high molecular substances in general require the study of the weak intermolecular forces which are determined by the surface of the molecule rather than directly by its internal constitution, and the same is true for the mesomorphic states of matter.

Acta is intended to offer a central place for publication and discussion of all research in this vast and ever-expanding field. It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features. Ever since crystals became the object of scientific investigation it has been felt that they are the most precisely defined form of matter, and that the understanding of their atomic structure introduces clarity and detail into concepts which must in other cases be expressed in more general terms. This is particularly apparent in all types of diffraction experiments, but it is also true for elastic, optical, electric, magnetic and thermodynamic properties, and the whole field of crystal structure may be regarded as the ultimate development of stereochemistry, amplified by a wealth of quantitative geometrical information.

Acta does not aim at diverting fundamental physical and chemical papers from the journals established for these sciences. It is, however, felt that a considerable body of investigations on crystalline and kindred substances would find a more appropriate place in a journal devoted to the detailed study of individual substances by the various methods, and to the further development of these methods. It is hoped that *Acta* will fulfil this useful function. Boundaries between scientific journals will always be fluid. But, to give an example of what is meant, the promoters of *Acta*,

and their editors, feel that the discovery of neutron or electron diffraction in a crystal is undoubtedly better placed in a journal devoted to pure physics; the application of these diffraction effects to the study of the scattering by individual crystalline substances, however, would appropriately come within the domain of *Acta*.

The best scheme for the publication of scientific investigations is a problem of outstanding importance for the sound development of science, and is particularly acute in those fields which touch on many different branches of study. On the one hand the results of crystal investigations should be presented to physicists, chemists, mineralogists, metallurgists and biologists in a form which enables them to grasp readily the implications for their sciences; they are not interested in the details of the methods by which the results have been achieved, and if such details are published in the existing journals, the majority of the readers may not be prepared to follow the argument. On the other hand, it is essential that the methods by which the results have been gained, and the data on which they are founded, should be fully published so that they may be subjected to the expert criticism necessary to assess their reliability. *Acta*, in trying to reassemble the crystallographic work now scattered through a great variety of journals and to give it full expression, should fulfil an important function in the general mechanism of scientific publication. It is frankly intended to be the main journal for experts in crystallography the world over. It is hoped that all important new lines of research will be represented in it, and that *Acta* will focus international discussion of problems of crystallography.

As regards organization, *Acta Crystallographica* is breaking new ground by belonging to the crystallographers themselves, being the property of an International Scientific Union. The INTERNATIONAL UNION OF CRYSTALLOGRAPHY was established in 1947 after preparations initiated at the meeting of crystallographers from many parts of the world held in London in July 1946 on the invitation of the X-ray Analysis Group of the Institute of Physics under the Chairmanship of Sir Lawrence Bragg. At this meeting a Provisional International Crystallographic Committee was formed consisting of some thirty of those present, and this in turn charged one of its Sub-Committees to take the necessary steps for the formation of a Union of Crystallography and for the publication of a journal, the editors of which were nominated at the meeting.

As a result of this, Statutes of the Union were prepared and approved by the Provisional Committee with their acceptance by the International Council of Scientific Unions on 7 April 1947 the Union of Crystallography came into being. Pending the first General Assembly of the new Union, the Provisional International Committee represents the Union, and the Sub-Committee formed at the London meeting serves as its provisional Executive Committee.

The question of arrangements for a centre of publication of *Acta* was very carefully considered; specifications for the printing were drawn up and tenders invited from firms in various European countries and in the U.S.A. The final decision to entrust the printing to the Cambridge University Press was governed largely by considerations of convenience of editing and publication. The Cambridge University Press is charged with the printing and distribution of *Acta* in accordance with the wishes of the Union. Much to the satisfaction of the Provisional Committee, the international character of the arrangements for *Acta* has been enhanced by the offer of the American Institute of Physics to collect subscriptions in the United States of America, its territories and possessions, in Canada and in Mexico.

It has been agreed to fix the subscription at £2. 10*s*. 0*d*. or $10 per volume, and to ask for subsidies in order to keep the price at this level. It is hoped that this moderate price will ensure a large number of subscribers. Subsidies have been obtained from U.N.E.S.C.O., from British and American firms, Research Associations, and other scientific bodies. This is not the place to list these contributions, but we most gratefully express the sincere thanks of the promoters, the editors, and the readers of *Acta* to those whose moral and material help has made possible the production of this journal.