SYMPOSIUM ON X-RAY STUDIES OF SUBSTANCES OF HIGH MOLECULAR WEIGHT[1]

INTRODUCTION TO THE SYMPOSIUM

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Twenty-six years have elapsed since W. H. Bragg and W. L. Bragg reported the first determination of the structure of a crystal with the aid of x-rays. Although the fundamental principles of the interaction of x-rays and crystals remain the same, there have been great improvements both in the technique of obtaining the data and in the technique of interpreting them. The structural details of complex organic molecules can now be successfully studied, the results checking well, where comparison is possible, with those obtained by other methods, such as electron diffraction, band spectrum, and dipole moment studies.

In all of the earlier x-ray diffraction work and in much that is done today, the x-ray data are used to study structural *regularities*. Nowadays, however, they are also being used, more and more, to give information regarding the *irregularities*—for example, random replacements of one kind of atom by another, oscillations and rotations of atomic groups and even of whole molecules, irregular distributions of alternative atomic arrangements having practically the same energy, and molecular orientation and structure in fibers and other not entirely crystalline materials. X-ray methods are not ideally suited to such studies and in many cases cannot tell us the whole story, yet they do furnish a certain amount of information which is at present obtainable in no other way. In order to use the x-ray data to the fullest extent, it is usually also necessary, with the more complex materials, to utilize information from various other fields and to reason to some extent by analogy with other comparable structures. This is, of course, quite proper and good scientific practice, provided it is done with sufficient care.

[1] This Symposium was held at the Ninety-eighth Meeting of the American Chemical Society in Boston, Massachusetts, September, 1939, under the auspices of the Divisions of Physical and Inorganic Chemistry, Colloid Chemistry, Organic Chemistry, Paint and Varnish Chemistry, and Rubber Chemistry of the American Chemical Society.

As the structures being studied become more complicated and as the necessity for including evidence from other sources increases, the conclusions reached depend more and more on the judgment of those drawing them. As a rule, non-specialists in the field can no longer judge adequately the validity of these conclusions by an inspection of the papers reporting the work. Moreover, for reasons of rigor and conciseness, the methods and frequently—indeed, almost invariably—even the results are reported in language which is unintelligible to the average reader.

Largely for these reasons, this symposium has been arranged. It brings before you some of the more important results which have been obtained with the aid of x-ray diffraction.

X-ray methods can be applied to very diverse problems. Those who work in the field often see applications to problems which, at first sight, are quite unrelated. This is especially true of industrial applications. It is hoped that valuable ideas and suggestions will be obtained from a perusal of these papers. The scope of the symposium is restricted to studies of substances of high molecular weight. These include such materials as rubber, cellulose and its derivatives, synthetic linear polymers, and proteins, in all of which x-ray evidence is of considerable technical as well as theoretical interest. Proteins are of considerable interest to biologists.

Although the papers treat primarily of substances composed of what we might call "*giant* molecules," some do, of course, discuss researches on substances composed of *small* molecules, whenever these help to furnish a suitable background of information.

Strictly speaking, most minerals—one might even say most inorganic compounds—should perhaps be included in the term "substances of high molecular weight." In this symposium, however, the discussion of inorganic substances is limited to glasses. These possess certain elements of irregularity which make the problems involved in the interpretation of the x-ray data similar in many respects to those met with in work on the other substances to be discussed.