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Preface

When von Laue and his assistants produced their first smudgy X-ray diffraction photographs in Munich in 1912 they could not have known of the developments that would follow and the impact that these would have on such a wide range of science. Structural crystallography, the ability to find the arrangement of atoms inside crystals, has advanced over the years both theoretically and experimentally. Technical advances, such as the development of computers both for control of instruments and for complex calculations, and also the advent of high power synchrotron X-ray sources have all played their part.

In this book we bring together all the methods that have been and are being used to solve crystal structures. We broadly divide these methods into two main classes, *non-physical* and *physical* methods. In the first category we place those methods that depend on a single set of diffraction data produced by the normal Thomson scattering from the individual atoms. The Patterson methods and direct methods described in chapters 2 and 3 respectively are non-physical methods. In chapter 4 the basic principles are explained for two physical methods – isomorphous replacement, which combines the data from two or more related compounds to obtain phase information, and anomalous scattering, which uses data at wavelengths for which some of the atoms scatter anomalously, i.e. with an amplitude and phase differing from that given by the Thomson process. In chapter 5 the method of isomorphous replacement is explored in much greater depth and in chapter 6 the same is done for anomalous scattering. It will be seen that some of the most effective ways of using *physical* data are in conjunction with *non-physical* methods, in particular direct methods, although Patterson function ideas also come into one successful technique for using anomalous scattering data.

The outcome of physical approaches, particularly when applied to

macromolecular structures, is that phases are found only for low resolution data although data at higher resolution might be available. This requires the techniques of phase extension and refinement which are described in chapter 7. Here we bring in some material slightly off the beaten track of conventional X-ray crystallography concerned with the solution of crystal structures by a combination of electron microscopy and diffraction and also the study of crystals with pseudosymmetry of various kinds.

In chapter 8, the final chapter, we describe what may be considered the most physical of all methods, which exploits the dynamical scattering process to acquire phase information. One of the helpful features of X-ray diffraction is that dynamical scattering effects are weak and this makes the connection between the observed data and the electron density in the crystal much more direct. It is therefore paradoxical that by doing very refined and accurate experiments to detect dynamical scattering effects one can go a long way towards solving the phase problem, the basic problem of structural X-ray crystallography.

We hope that this book will be found useful by working crystallographers and, in particular, those, such as graduate students, who are being introduced to the problems of solving crystal structures for the first time. For our readers who are at the beginning of their crystallographic studies we have given in chapter 1 an introduction to the field, sufficient to give comprehension to what follows without the pretence of being a complete treatment. Indeed we would not pretend that within the confines of a book of modest size we have covered exhaustively all the topics with which we have dealt. If we can give understanding and point the way to further reading and study where required then we shall have achieved our purpose.