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Preface to the Second Edition

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## 1 Introduction

Molecules come in a bewildering variety of shapes and sizes, and with a huge diversity of structural complexity. From the simplest homonuclear diatomic molecules such as  $H_2$  to macromolecules such as haemoglobin containing many thousands of constituent atoms, the complexity of any molecule derives from the large number of potential constituent atoms, the types of bonds which hold the nuclei together and the degree to which the atoms arrange themselves into symmetric structures. Whilst the universe is generally said to prefer to favour increasing disorder as the natural order of things, nature has a habit of creating molecules of considerable structural order and symmetry. Indeed, the extent to which any given molecule can be regarded as either unsymmetrical and disordered in its form or symmetrical, ordered and, yes, beautiful, is usually directly correlated with the efficiency with which it carries out its chemical functions.

Molecular bonding is absolutely fundamental to all aspects of chemistry and it is the nature of the interactions that exist between nuclei, both weak and strong, which defines the types of structures that can be constructed from the atomic building blocks. Our understanding of chemical structure derives to a great extent from the theory of the chemical bond and, in particular, from the foundations laid by the development of quantum theory and quantum mechanics in the early part of the 20th century. However, it also depends critically on our ability to determine molecular structures through experiment.

This book presents a number of different experimental strategies to determine the geometrical arrangement of atoms in space that make up a particular molecule. The choice of which technique to use depends on a number of factors such as whether we are dealing with a crystalline, liquid or gas phase sample, whether the molecule is small or large, how symmetric it is and whether we need precise determination of bond lengths and bond angles. In cases where we need more general structural information, we might be interested, for example, in the structural relationship between functional groups in an organic molecule, or the arrangements of ligands around a metal centre in a transition metal complex or indeed in the way in which a cardiovascular drug molecule might bind within the protein cavity in haemoglobin.

Most of the methods described in this book rely on the interaction of photons or electrons with the molecule of interest. Those that use photons exploit whichever regions of the electromagnetic spectrum are appropriate to the probing of rotational,