

1 Introduction

Structural chemistry or *stereochemistry* is the science of the structures of chemical compounds, the latter term being used mainly when the structures of molecules are concerned. Structural chemistry deals with the elucidation and description of the spatial order of atoms in a compound, with the explanation of the reasons that lead to this order, and with the properties resulting therefrom. It also includes the systematic ordering of the recognized structure types and the disclosure of relationships among them.

Structural chemistry is an essential part of modern chemistry in theory and practice. To understand the processes taking place during a chemical reaction and to render it possible to design experiments for the synthesis of new compounds, a knowledge of the structures of the compounds involved is essential. Chemical and physical properties of a substance can only be understood when its structure is known. The enormous influence that the structure of a material has on its properties can be seen by the comparison of graphite and diamond: both consist only of carbon, and yet they differ widely in their physical and chemical properties.

The most important experimental task in structural chemistry is the *structure determination*. It is mainly performed by X-ray diffraction from single crystals; further methods include X-ray diffraction from crystalline powders and neutron diffraction from single crystals and powders. Structure determination is the analytical aspect of structural chemistry; the usual result is a static model. The elucidation of the spatial rearrangements of atoms during a chemical reaction is much less accessible experimentally. *Reaction mechanisms* deal with this aspect of structural chemistry in the chemistry of molecules. *Topotaxy* is concerned with chemical processes in solids, in which structural relations exist between the orientation of educts and products. Neither dynamic aspects of this kind are subjects of this book, nor the experimental methods for the preparation of solids, to grow crystals or to determine structures.

Crystals are distinguished by the regular, periodic order of their components. In the following we will focus much attention on this order. However, this should not lead to the impression of a perfect order. Real crystals contain numerous faults, their number increasing with temperature. Atoms can be missing or misplaced, and dislocations and other imperfections can occur. These faults can have an enormous influence on the properties of a material.