

Physical Methods in Inorganic Chemistry

Applications of X-ray diffraction: Single Crystals and Powders - Dr. H. Kooijman

X-ray diffraction is a powerful tool to investigate crystalline materials at the atomic level. In this contribution the background of diffraction studies will be briefly discussed, but the main focus will lie on using the information that can be obtained from a diffraction study. We will explore the possibilities of both single-crystal diffraction and powder diffraction. The result of a **single-crystal study** is a list of accurate atomic positions which allows a detailed geometric analysis of molecular structure and crystal packing. The information that can be extracted varies from simple bond lengths to the connectivity of the hydrogen bond network. Some time will be spent on tools to judge the significance of the obtained geometric parameters. **Powder diffraction** studies are used for various purposes. Although structure determination from powders is far from trivial, it is used more and more in those cases where single crystals are not available. The obtained structure is in general less accurate than that from a single-crystal study, but can still be the basis of detailed geometric analyses. Another popular application of powder diffraction is that of fast identification or verification, not only of pure compounds but also of mixtures. Several techniques to quantify the composition of mixtures will be discussed. Finally, the possibility to perform powder studies under non-ambient conditions will be briefly discussed.

Prerequisites: a basic knowledge of X-ray diffraction is helpful but not necessary.