PREFACE

Crystallography as a subject in research and university teaching lacks clear definition and boundaries. It is a typical in-between discipline. Crystallographers may have basic education in physics, chemistry, mineralogy, biochemistry, metallurgy or material sciences. The original meaning of the term crystallography "to describe a crystal" placed the discipline besides mineralogy. The advent of X-rays changed the general understanding of crystallography to "crystal structure determination" as the mean vocation for a crystallographer. But the automatization in solving structures has widely discredited "chemical crystallography" to "service crystallography." Good many of our honored colleagues in preparative chemistry departments seem to be misled by the term crystal structure analysis which they quite simply interpret as chemical analysis. The diffractometer is perhaps the easiest way to make sure what your reaction produced provided it gave a single crystal. The data analysis then gives the answer what the initial intention was when the preparation started. "The computer told me that the space group is correct" is the basic knowledge of symmetry required. It is evident that the future of crystallography will not be found in that direction, despite the fact that solving molecular crystal structures and relating them to the conformation in solution constitutes an important task for crystallography.

It is certainly more difficult to interpret NMR-data of molecules in solution but is therefore the result scientifically more relevant than a crystal structure? X-ray structures are likely to represent a major conformer in solution and are likely to explain spectra. The answer cannot be a fight of methods but an approach to use spectroscopy and diffraction simultaneously as complementary methods. This holds equally well for all types of calculations of structures based on energy minimization whether it is for molecules or for the solid state.

The inherent relation between structure and physical or chemical properties should constitute the basis of crystallographic thinking. The crystallographer should explain concisely how the data obtained by crystal structure analysis is related to chemical, physical or biological properties of the solid.

Structure here is not just the ideal arrangement of atoms in one of our 230 space groups, it includesalsothedeviation from ideality, reality makes life interesting; an ideal person isas boring asan ideal crystal. Defects, phase changes, surfaces are the basis of the properties of solids. Thus crystallography has to include the study of the amorphous and glass states, the crystallization process and all kinds of intermediates like plastic, liquid and quasi crystals, crystalline polymers and other kinds of materials. The periodicity and the symmetry of the internal structure is reflected by the periodicity of properties. Focus is at present on material sciences which inherently ask for crystallographic methods. Symmetry is a major principle in nature and art, it is the basis of crystallographic thinking.

The methodological base of the investigation is the diffraction process, whether particles like electrons and neutrons orx-raysfrom a tube ora synchrotron areapplied. The complementary use of neutrons stimulated X-ray research, nicely documented by the X-N techniques for deformation density studies or by the role of neutron scattering in polymer research. Achievements likethe profile analysis of powder pattern (Rietveld method) were first developed for neutrons and afterwards adapted to X-rays. The very successful isotopic replacement technique is, however, unique for neutrons.

Synchrotrons will not equally replace the X-ray tube, they will extend its application and stimulate new needs in the home laboratories, like rotating anodes, higher resolution instruments or position sensitive detector systems. The research centers which were created around a powerful source of either neutrons or synchrotrons are an ideal meeting place. Crystallographers will meet their colleagues from other disciplines around facilities of common interest. This may allow to include new techniques like EXAFS or XANES and to combine them with the diffraction experiment. These big facilities can no longer be operated as national laboratories. European solutions have been found for the neutron scattering community with the Institut Laue-Langevin and the ESRF for synchrotron radiation both at Grenoble (France). A next generation neutron source can only be built in a supranational context. The important question then is not whether a pulsed or a steady state source is needed but how is the maximum number of neutrons available.

Another important challenge for the future development in our field is computing. Up to now only very few institutes are directly connected to information centers and use data bases. An exchange of data, e.g. raw data from a synchrotron source, is still in its infancy. When the potential usefulness of molecular modelling was recognized by industry only very few young crystallogra-. phers were trained to do the job.

What does all this mean to a scientific entity which is the group of crystallographers? To my understanding the gates should be wide open to all neighbouring disciplines, towards research centers which provide excellent facilities and towards all kinds of methods giving information on the solid state. This information should be combined with the basic knowledge of symmetry and fundamental laws of diffraction physics which constitutes our traditional domain.

Thus an association of crystallography ought to include scientists as different as chemical crystallographers, mathematicians interested in the laws of symmetry, biochemists solving large structures or material scientists.

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