

P09**Progress in the application of synchrotron radiation in chemistry and biology**

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It is well known that the use of synchrotron radiation has revolutionised structural biology and is responsible for the exponential growth of known macromolecular structures in the Protein Data Bank. So one may wonder if continued progress is possible. The recent developments of beamlines for macromolecular crystallography at the ESRF have had the purpose to make them highly automated. This has enabled the users to screen a multiplicity of samples to find the best suited crystal for data collection. The use of crystallization robots tends to yield smaller crystals, which creates an increasing demand for beamlines with small beams to be used for the diffraction experiments. These developments make it possible to study larger and more complex biological systems, bringing the structural biology closer to the studies of soft condensed matter. We can also observe an increasing interest to complement the diffraction studies with complementary methods like small angle scattering and imaging. The use of nanometer sized X-ray beams is also in demand for investigations of chemical systems. The use of nanosized beams opens possibilities for an unprecedented spatial resolution that open new scientific possibilities in materials science, soft matter chemistry and the characterization of complex chemical systems. The possibility of conducting the experiments at the synchrotron on samples under different thermodynamic conditions has stimulated an avenue of studies of chemical systems under extreme conditions. There is a similar interest in employing the time structure of synchrotron radiation in time resolved studies. The trends in the application of synchrotron radiation in chemistry and biology will be described and illustrated by recent scientific achievements [1].

[1] Highlights 2005, European Synchrotron Radiation Facility.

P10**Charge, spin and momentum densities: different faces of this same nature**

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Charge, spin and electron momentum density distributions were of great interest of crystallographers since early days of the crystallographic and magnetic structures investigation, and the studies made with the use of the Compton spectroscopy. The main ingredients in the structure refinement techniques were form-factors which were calculated for free atoms, next for molecules and solids by means of more and more sophisticated methods. When it became clear that all the properties of solids can be derived from the knowledge of a functional of the charge and spin density distributions, the motivation for studies of these distributions was strengthened. However, it soon turned out that precise measurements of form-factors require special carefulness, so many methods of reconstruction of the density distributions were and are still developed. An interesting turn in thinking of the density distributions was introduced with the advent of so-called topological analysis which enabled, at least theoretically, to infer a lot of microscopic details from the measured charge density distribution, and in particular emphasize the nature of chemical bonds. The main difficulty, however, was connected with the fact that usually a number of outermost electrons deciding about the bonds is much smaller than the number of core electrons, and the corresponding signals from the valence electrons are weak or nearly zero in the case of strongly delocalized electrons. Magnetic neutron diffraction turned out to have many advantages in such cases because the signals measured were connected mainly with one, at least very few, shells responsible for the magnetism of the substance. However, even in this case, the signals from the outermost s-electrons were hardly seen. Nevertheless, good evidence of covalency effects were observed, and recently a lot was learned about the nature of magnetism in molecular crystals. The magnetic form-factor analysis serves also as a very good tool enabling to separate magnetic moments into their spin and orbital components. In both, X-ray and neutron diffraction, the analysis of the charge or spin densities encountered a difficulty connected with often unknown phases of the wave functions which were probed only through the squares of their absolute values. On the other hand, Compton spectroscopy offered much more direct access to the electronic wave functions. The electron momentum density which is measured by the Compton scattering technique is connected with the squares of the Fourier transforms of the wave functions, which makes the result highly sensitive to the details of the wave functions. This in turn makes this technique extremely valuable in showing the correctness of the assumed crystal potentials and importance of the electron-electron correlations whose description goes beyond single-electron approximation. It does not seem possible to obtain full information on the electronic wave functions in a system from the charge and spin densities only. All groups who are studying the charge, spin or momentum density distributions try to reach the same goal - to catch the nature of crystal potentials, bonds etc. However, the techniques used are bringing information somewhat different and there were so far very few successful attempts to combine this information and make full use of it.