PhD Project

Intermolecular interactions studied by liquid- and solid-state NMR spectroscopy and advanced quantum-chemical computations

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Modern chemistry, biology and materials science are based on the knowledge of structure on the molecular level. The relationship between molecular structure and physico-chemical and biological properties is the central paradigm of current science. The weakest point of current structural analysis is the lack of techniques suitable for accurate determination of hydrogen atom positions and techniques suitable for studying disordered materials. A prominent example is X-ray crystallography, which is the most widely used technique for determination of structures with atomic resolution but there are limitations to this technique. Hydrogen atoms are very difficult to characterise by X-ray diffraction, therefore, structural phenomena that include hydrogen atoms, such as tautomerism or co-crystal/salt formation, are challenging for this method. Another well-known limitation of diffraction methods is that they require a highly ordered crystalline sample.

An alternative experimental technique for atomic-level characterisation of organic molecules is NMR spectroscopy. Hydrogen atoms possess the most sensitive nuclei for NMR and solid-state NMR spectroscopy (SS-NMR) does not require a long-range order in the studied materials and is, therefore, suitable for characterisation of disordered and amorphous samples.

The aim of the PhD project is studying intermolecular interactions of biologically relevant molecules and other compounds/materials by a combination of NMR spectroscopy and advanced quantum-chemical calculations. A particular emphasis will be given to the influence of intermolecular interactions on tautomeric equilibria and to the investigation of the structure and dynamics of disordered solids. Intermolecular interactions responsible for the structure, structural transformations and dynamics of molecules will be investigated.