Solid state NMR – molecular dynamics and dynamics of hydrogen bond research group (dr Piotr Bernatowicz)

The research of NMR group is focused on widely defined molecular dynamics, both in the solid and in the liquid states. The methods of nuclear spin relaxation and numerical lineshape analysis are extensively exploited as a basic tool. Most of the advanced software used to this end is written in-house by the staff of the laboratory.

The detailed topics of group’s research interest comprise:

1. Further experimental verification of the Damped Quantum Rotation (DQR) theory developed by Prof. Sławomir Szymański, one of the group members. This theory describes both the coherent and stochastic dynamics of molecular rotors (like the methyl group) in a consistently quantum mechanical way. In the DQR approach, the random jump model normally used to describe the stochastic motions of such objects appears as a limiting case realized only for rotors strongly coupled to their condensed environment.

2. Investigation of both global and internal molecular dynamics in isotropic liquids. In cooperation with Prof. Jozef Kowalewski from Arrhenius Laboratory of Stockholm, we derived the theory which links some observables determined in the course of NMR experiments (so-called spectral densities) to the details of molecular dynamics. This allows for accurate determination of rotational diffusion tensors of molecules and mechanisms and rates of the internal motions which accompany global molecular tumbling e.g. methyl group reorientation, proton jumps, ring wagging etc. We check how our theory works on model compounds: cyclodextrins, porphycene, 1,8-(bisdimethylamino)naphthalene etc.
3. Investigations of the processes induced in molecules by laser light. This project is carried out in cooperation with the Department of Photochemistry and Spectroscopy of IPC PAS. It involves coupling of laser and NMR spectrometer in order to perform NMR detection of the response of the sample excited by UV/VIS light. The excitation may cause proton transfer, charge transfer associated with a ring twist (so-called TICT effect), generation of carbenes followed by a chain of subsequent chemical reactions initiated by these reactive species etc.

4. Prof. Helena Dodziuk extends her studies of cyclophanes. It involves two types of problems:
   a) Studies of two groups of compounds: [2.2]- and [2.2.2] cyclophanes with unsaturated bonds in the bridges. NMR and UV spectra were measured and the structure and chemical shifts and coupling constants were calculated. In order to determine more accurately NMR parameters and to measure almost all $J_{HH}$ values, the spectra were analyzed numerically. An example of the fitting for a fragment of the proton spectrum is shown.

   b) In addition, a study of the [m,n]cyclopane series is carried out allowing one to analyze, in case of $m \neq n$, the interaction between two aromatic rings when they are inclined in comparison to their parallel orientation for $m = n$.

5. In collaboration with Dr. Tatiana Korona from the University of Warsaw, Prof. Helena Dodziuk performs calculations using SAPT method for an opened carbon nanotube $C_{50}H_{10}$ (which was recently synthesized) with numerous molecular and noble gas guests X to analyze their stability with the aim to give clues to synthetic chemists which X@$C_{50}H_{10}$ complexes are plausible targets.