TIFR Centre for Interdisciplinary Sciences
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Seminar

Development and Application of Solid-State Nuclear Magnetic Resonance Methods: From Biomolecules to Materials

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Solid-state NMR is a versatile analytical technique to study structure and dynamics of a diverse range of molecules without placing any restriction on the physical properties of the sample (Crystallinity, solubility etc.). Despite the introduction of techniques such as Magic Angle Spinning (MAS) and decoupling as early as 1950's the field of solid-state NMR has been hampered by limitation in resolution and sensitivity. This presents a major hurdle in study of number of samples by solid-state NMR and will be highlighted by a pilot study on multidrug transporter EmrE. Despite, such limitations, it is still possible to obtain site-specific information, in this case we could identify the binding sites in the multidrug transporter.

Over last 15 years, rapid development in NMR methods and hardware have addressed the issues of resolution and sensitivity, specifically, by introduction of fast and ultra-fast MAS, improved decoupling schemes, new sample preparation protocols, creative labelling, higher dimensional spectroscopy etc. We have used isotope-labelling strategies combined with proton detection to overcome problems of resolution and sensitivity in the solid-state. Through these modifications, the quality of spectra in the solid-state have become comparable to those obtained from solution-state NMR. This has enabled structure determination of proteins with only about few hundred microgram of protein sample at 100 kHz MAS frequency. This approach has also been successfully used in probing new applications such as a) studying dynamics of proteins in the solid-state and b) identifying and characterizing hydrogen bonds in proteins. The study on dynamics discusses similarities and differences between dynamics of a globular protein in the solution and crystalline state while hydrogen bond study localizes protons in hydrogen bonds and subsequently uses them as structural restraints in larger protein assemblies.

The second part of the presentation will briefly focus on a new second-order recoupling and a new decoupling sequences developed exclusively for fast Magic Angle Spinning (MAS).

In the end, I will also present some results where solid-state NMR from different static magnetic fields can be combined to develop an understanding of mechanical properties of polyolefinic polymer (e.g. such as polypropylene) in terms of their chemical and physical structures.

Tuesday, August 5th 2014

11:30 AM (Tea/Coffee at 11:15 AM)

Seminar Hall, TCIS