Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

Methods Development and its applications in NMR

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Solid-state NMR is a very flexible and powerful technique for elucidation of geometry and dynamics information on a variety of samples. However, there is still need to overcome sensitivity and resolution aspects. Our approach involves the improvement of heteronuclear spin decoupling efficiency at high magic-angle spinning (MAS) frequencies. For this, a unified strategy[1] of two-pulse based heteronuclear decoupling for high-spinning frequencies and low-power radio-frequency irradiation in solid-state MAS NMR is presented which incorporates simultaneous time and phase modulation. Decoupling sequences like TPPM, XiX and rCW turn out to be specific solution of this approach. This approach, shown schematically in Fig.1, not only highlights the existing solutions but also generates new solutions for efficient decoupling.

A recent report[2] described the macroscopic picture of the mechanism for the crystallization of perovskite i.e. the dissolution of colloids towards the formation of single crystals. However, the molecular picture is still not clear. We have tried to understand the role of solute-solvent interaction towards the formation of single crystals which is also an important parameter.

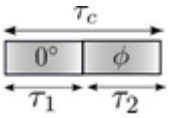

Fig.1: Unified two-pulse decoupling scheme which forms the basic building block of most decoupling sequences

References:

1. A. Equbal, M. Bjerring, P. K. Madhu, N. C. Nielsen. A unified heteronuclear decoupling strategy for magic-angle-spinning in solid-state NMR. J. Chem. Phys. 184201-8, 2015.
2. P. K.Nayak, D. T. Moore, B.Wenger,S. Nayak, A. A. Haghihirad, A. Fineberg, N.K. Noel, O. G.Reid, G. Rumbles, P. Kukura, K.A.Vincent, H.J.Snaith. Mechnism for rapid growth of organic-inorganic halide perovskite crystals. Nat.Comm., 65(3): 1-8, 2016.

Tuesday, Apr 03rd 2018

02:30 PM (Tea/Coffee at 01:30 PM)

Seminar Hall, TIFR-H