Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally Mandal, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Improving ^{1}H resolution at fast Magic Angle Spinning frequencies using Combined Rotation and Multiple Pulse Sequences

Mrudula Mangesh Nikam

TIFR, Hyderabad

^{1}H detection is highly sensitive due to the high gyromagnetic ratio of ^{1}H, but it also results in strong ^{1}H-^{1}H dipolar couplings in solids. These strong dipolar couplings result in faster relaxation for proton transverse magnetisation and consequently lead to broad resonances and poor resolution. Advancements in magic-angle-spinning (MAS) probe technology have enabled the acquisition of high-resolution spectra by mechanically rotating the sample aligned at the magic angle, which removes these dipolar couplings (to the first order). Nevertheless, the optimal resolution achieved at maximum spinning speeds remains much inferior to that attained in solution NMR. Combined rotation and multiple pulse sequence (CRAMPS) methods have been applied to achieve high resolution at spinning speeds of 62.5 to 80 kHz. However, the improvement in resolution is limited by rf inhomogeneity dependent heterogeneous broadening. In this work, we present a homonuclear decoupling technique based on super-cycled PMLG pulses with different phase ramps, which results in factor of 1.3-2.0 improvement in proton resolution as well as 2-4 times increment in proton coherence lifetimes, while maintaining high scaling factors (≥0.8) at 60 and 95kHz MAS. We further investigate the role of phase ramp in homonuclear decoupling performance and demonstrate that efficient decoupling can also be achieved using a simpler z-rotation-based approach without a phase ramp. Comparable improvement in resolution is obtained with and without phase ramp. We show implementation of these methods on standard peptide f-MLF, standard protein GB1(6kDa) and 326-residue cytoskeletal protein ParM(36kDa) in its filamentous state. These methods provide spectral resolution comparable to that achieved at higher MAS frequencies while benefiting from the larger sample volumes and corresponding sensitivity of larger rotors.

Tuesday, Oct 27th 2026

14:00 Hrs (Tea / Coffee 13:45 Hrs)

Auditorium, TIFRH