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Probing Noncovalent Interactions by Fast Magic-Angle Spinning NMR at 100 kHz and More

Thursday 18 September 2025 10:00 (30 minutes)

Molecular-recognition events play a key role in biology and chemistry and are driven by noncovalent interactions, such as hydrogen bonding or dispersion interactions. Proton nuclear spins in NMR experiments serve as highly sensitive reporters for such weak chemical interactions. Only recently, the technically achievable magic-angle spinning (MAS) frequencies have become high enough to efficiently average out the dipole couplings in the dense proton dipolar network, which otherwise led to rather broad and unresolved 1H resonances in solids blurring the information on noncovalent interactions.

I will discuss the benefit of proton-detected solid-state NMR experiments at MAS frequencies of 100 kHz and more and at high static magnetic-field strengths in chemical and biological applications emphasizing effects of weak interactions. The examples I will focus on range from hydrogen-π and cation-π interactions in calix[4]arene-based lanthanide complexes to hydrogen bonding in nucleic-acid binding to large ATP-fueled motor proteins. Of particular interest in this vein is to explore the temperature dependence of proton chemical-shift values, which can be diagnostic for hydrogen-bond formation.

Keywords

This abstract is submitted for....

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Primary author: WIEGAND, Thomas (RWTH Aachen University & Max Planck Institute for Chemical Energy Conversion)

Presenter: WIEGAND, Thomas (RWTH Aachen University & Max Planck Institute for Chemical Energy Conversion)