PhD Position: Cryogenic molecular dynamics and magic-angle spinning NMR

NMR can provide detailed information on the local structure and dynamics, with atomic resolution, in a wide temperature range. For many nuclei, improved resolution is achieved by rotating the sample about the "magic-angle". Magic-angle spinning (MAS) can resolve inequivalent chemical sites. In the UK, a cryoMAS system is available uniquely in Southampton.

Molecular motions are temperature dependent. By lowering the temperature, some motions are slowed down or even frozen, but many interesting motions involving light-weight molecules or molecular fragments, like CH3 groups, water molecules and hydrogen, persist even at very low temperature. These motions are very unhindered and fast, and they are often poorly described by classical physics. This makes it difficult to understand them in details at room temperature.

This project will study the physics of non classical, low temperature motions and their impact on NMR, using cryoMAS, to understand and predict quantitatively the factors controlling the behaviour of nuclear spins at low temperature and the influence of the molecular environment on them.

The main focus will be on spin diffusion, tunnelling motions, dipolar order and exotic phenomena like the Haupt effect. The Haupt effect has the potential to vastly increase the thermal polarization signal, since the rotational energy levels of the methyl group are at the origin of this effect.

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The Centre for Doctoral Training in Integrated Magnetic Resonance (iMR) is a collaboration between researchers at the Universities of Warwick, St Andrews, Southampton, Aberdeen and Nottingham.