PhD Position: Cryogenic NMR spectroscopy of molecular quantum rotors

Many interesting and technologically important phenomena take place in the cryogenic temperature regime, i.e. below the boiling point of liquid nitrogen (77 K). Examples include superconductivity, quantum tunnelling and quantum molecular rotation. This project concerns the study of low-temperature quantum phenomena by nuclear magnetic resonance (NMR). We will use low-temperature NMR equipment that has only recently become available and which allows, for the first time, high-resolution NMR spectra to be obtained in the cryogenic regime. The aim is to obtain unique information on phenomena such as quantum tunnelling and superconductivity, with chemical site selectivity.

One particularly interesting target for these studies is provided by molecular quantum rotors. These are molecules which are free to rotate at low temperatures, and whose motion must be described by quantum mechanics. Examples are provided by the supramolecular system H2@C60, which comprises dihydrogen molecules (H2) entirely encapsulated in fullerene cages (C60). The hydrogen molecules rotate freely inside the cage but cannot escape. These remarkable systems may be synthesized by organic chemistry methods. We have full access to these compounds in our group through international collaborations with Kyoto University (Japan) and Columbia University (New York, USA).

In this project you will study the behaviour of these quantum rotors using low-temperature NMR. You will study the NMR properties of a variety of such systems, and interpret the NMR properties using theoretical descriptions of the nuclear magnetism and the quantum molecular motion.

We are developing concepts in which such molecular rotors are used as agents for the strong enhancement of NMR signals. This would have important consequences for a range of important fields, such as magnetic resonance imaging and chemical spectroscopy. This project offers an opportunity to participate in a novel and interdisciplinary research area. The project will be based at Southampton University, where there is equipment available for cryogenic magic-angle-spinning NMR at temperatures down to 13 Kelvin. The project will also involve collaborations with the Universities of Nottingham and Warwick.

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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.