PhD Position: Developing Solid-State NMR Methods Utilising Residual Dipolar Couplings to Determine Distances in Multi-Spin Systems

The power of magnetic resonance to probe structural details with atomic resolution lies principally in the inherent dependence of the dipolar coupling between two spins on their separation to the inverse cubed power. In NMR, dipolar couplings can be exploited to determine, for example, the three-dimensional structure of a protein or interactions between pharmaceutical molecules in a tablet. A particular challenge, however, is to determine key longer-range (> 4 Å) distances in multi-spin systems where the phenomenon of dipolar truncation means that the presence of strong dipolar couplings (corresponding to short distances, e.g., a one-bond C-C interaction) hinders the accurate determination of weaker dipolar couplings (corresponding to longer-range distances). The Warwick and Southampton groups have recently presented a novel approach that combines sample spinning slightly off the magic angle with a spin-echo experiment incorporating a doubly selective inversion pulse (Pileio et al Chem Phys Lett 456, 116, 2008): the two groups have recently shown that this approach allows distances of over 4 Å to be accurately determined in multi-spin systems (Thureau et al Phys Chem Chem Phys 2010 & Becker-Baldus et al PhysChem Chem Phys 13, 4514, 2011).

This project continues the collaboration between the Warwick and Southampton groups to further develop this methodology. The research program will combine experimental work using the high-field spectrometers in Warwick and Southampton with numerical densitymatrix simulations. A specific goal is to extend the applicability of the approach from the previously demonstrated application to 13C to determining 1H-1H dipolar couplings.

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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.