PhD Position: Developing Solid-State NMR Correlation Experiments for Half-Integer Quadrupolar Nuclei

In NMR, two-dimensional homonuclear and heteronuclear NMR correlation experiments are powerful techniques for identifying the through-space proximity or through-bond coupling of atoms via the *J* coupling or dipolar coupling of the atomic nuclei, respectively. Approximately two-thirds of all NMR-active nuclei have spin quantum number $I \geq 1$, and there are a number of important elements for which the only NMR-active nucleus is quadrupolar, e.g., boron, oxygen, sodium, and aluminium. For nuclei with spin quantum number $I \geq 1$, obtaining two-dimensional homonuclear and heteronuclear solid-state NMR correlation spectra with sufficient resolution is much more challenging as compared to for spin $I = 1/2$ nuclei because of line broadening (that is only partially removed by magic-angle spinning) due to the so-called quadrupolar interaction between the electric quadrupole moment of the nucleus and the electric field gradient.

This project will involve the development of new solid-state NMR correlation experiments, between either two half-integer quadrupolar nuclei or a half-integer quadrupolar nucleus and a spin $I = 1/2$ nucleus. The project is a collaboration between the research groups of Steven P. Brown (Warwick) and Sharon E. Ashbrook (St Andrews) and will combine experimental work using the high-field spectrometers in Warwick and St Andrews with numerical simulations of NMR experiments. For a recent example of such an approach, see the joint Warwick-St Andrews publication: Barrow et al., Phys. Chem. Chem. Phys. 13, 5778, 2011.

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