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Liquid-solid interface characterization of organometals grafted to cross-linked polymers using high-resolution Magic Angle Spinning NMR spectroscopy

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The structural characterization of organotin compounds that are grafted on insoluble cross-linked polymers has necessarily been limited to elemental analysis, infra-red spectroscopy and, in a few instances, solid state NMR spectroscopy. This has been an important bottleneck in the development of such systems, intended for use as heteregeneous catalysts, or as functionalised polymers for application in organic chemistry. We have addressed this problem with high-resolution magic angle spinning (hr-MAS) NMR spectroscopy. This technique borrows the *magic angle spinning* technique, well-known from solid-state NMR, to narrow down resonance lines to nearly liquid like line-widths, such that 1D and 2D high resolution NMR spectra may be applied for the detailed structure elucidation of the grafted compound in the solvent swollen polymer matrix.

The potential of this technique is demonstrated through the structural characterisation of various organotins grafted on divinylbenzene cross-linked polystyrene by means of a suitable linker. Suitable conditions for the application of hr-MAS NMR spectroscopy were identified using the 1H resonance line-widths of the grafted organotin moiety following swelling of the functionalised beads in 8 representative solvents. Following this, we used the presence of clearly identifiable tin coupling patterns in both the 1D 13C and 2D 1H-13C HSQC spectra, and the incorporation of 119Sn chemical shift and connectivity information from hr-MAS 1D 119Sn and 2D 1H-119Sn HMQC spectra, to provide an unprecedented level of characterization of grafted organotins directly at the solid/liquid interface. In addition, the use of hr-MAS 119Sn NMR for reaction monitoring, impurity detection and quantification and assessing coordination extension reveals its promising potential as a novel tool for investigating polymer grafted organotin compounds. The approach described here should be sufficiently general to be extended to a variety of other nuclei of interest in polymer supported organometallic chemistry.

1. Aaa, A., Bbb, B., Ccc, C. and Zzz, X. Y. *J. Am. Chem. Soc.* 2000, **115**, 0123-4567.
2. others….