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Strong-coupling induced damping of spin-echo modulations in magic-angle-spinning NMR: implications for J coupling measurements in disordered solids

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ABSTRACT

In the context of improving J coupling measurements in disordered solids, strong coupling effects have been investigated in the spin-echo and refocused INADEQUATE spin-echo (REINE) modulations of three- and four-spin systems under magic-angle spinning (MAS), using density matrix simulations and solid-state NMR experiments on a cadmium phosphate glass. Analytical models are developed for the different modulation regimes, which are shown to be distinguishable in practice using Akaike's information criterion. REINE modulations are shown to be free of the damping that occurs for spin-echo modulations when the observed spin has the same isotropic chemical shift as its neighbour. Damping also occurs when the observed spin is bonded to a strongly-coupled pair. For mid-chain units, the presence of both direct and relayed damping makes both REINE and spin-echo modulations impossible to interpret quantitatively. We nonetheless outline how a qualitative

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