Low-power broadband solid-state MAS NMR of $^{14}$N

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We propose two broadband pulse schemes for $^{14}$N solid-state magic-angle-spinning (MAS) nuclear magnetic resonance (NMR) that achieve (i) complete population inversion, and (ii) efficient excitation of the double-quantum coherence using low-power single-sideband-selective pulses. We give a comprehensive theoretical description of both schemes using a common framework that is based on the so-called jolting-frame formalism of Caravatti et al. 1, and which has been previously shown to be successful for developing low-power excitation pulse schemes for paramagnetic systems 2-4. This is a remarkably powerful description that summarizes the complex spin dynamics in a straightforward way, and enables us to design new pulse schemes for different applications.

Firstly we use this formalism to explain the conditions under which we may obtain complete spin population inversion using single-sideband-selective adiabatic pulses (S$^3$APs). In the best cases it is shown that complete inversion of the spinning-sideband manifold is obtained for a $C_Q$ that is more than an order of magnitude greater than the radiofrequency (RF) field amplitude.

We then exploit the full power of the jolting-frame formalism for $^{14}$N to develop a pulse scheme that excites $^{14}$N double-quantum coherences using low-power single-sideband-selective pulses. Excitation efficiencies of 30—50% are obtained using RF field amplitudes that are an order of magnitude lower than the $C_Q$. The scheme easily can be incorporated into other pulse sequences.

These pulses and irradiation schemes are evaluated numerically using simulations on single crystals and full powders, as well experimentally on ammonium oxalate at moderate (20 kHz) MAS, and glycine at ultra-fast (111 kHz) MAS.