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Generating and Exploiting Impossible Intermolecular Multiple Quantum Coherences in Solution NMR

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In the last few years, it has been discovered that samples with at least one concentrated component can grossly violate the predictions of conventional NMR theory in a wide variety of solution NMR experiments. Slightly modified conventional sequences, which should give absolutely no signal, instead give strong intermolecular cross-peaks and new transitions in the indirectly detected dimension. For example, the n-quantum CRAZED sequence ($\pi/2$-t_1-{gradient, length T}-$\pi/2$-{gradient, length nT}-t_2) generates resonances in the indirectly detected dimension with all of the experimental properties of intermolecular multiple-quantum coherences (iMQCs). The theoretical picture of these effects shows that the additional peaks come from dipolar interactions between distant spins in solution. The dipolar interaction between nuclei is proportional to $(3\cos^2\theta-1)/r^3$ where is the angle between the internuclear vectors and the applied magnetic field and r is the separation between the spins. In a liquid these intermolecular dipolar interactions have been safely ignored due to the molecular diffusion and sample symmetry. By breaking the uniform direction of the magnetization (usually gradient pulses) we can reintroduce effects of the dipole-dipole coupling between distant spins. The magnitude of the reintroduced couplings is comparable to a J coupling (2-3 Hz), hence is large enough to dramatically alter two-dimensional spectra, but not so large as to degrade resolution. This interactions can be handled in two superficially different waysclassical and quantum treatments.

We have recently developed the ability to calculate evolution in systems with both dipolar and J couplings [1,2], and the ability to handle three-dimensional structure (tissues with tumors; inhomogeneous broadening in very high field magnets) [3]. Here, we will show how intermolecular zero-quantum coherences (simultaneously flipping spins separated by 10μm-10mm in opposite directions) permits contrast enhancement for in vivo magnetic resonance imaging [4,5]. In addition, we will discuss work beginning at the National High Magnetic Field Laboratory using such coherences to produce sharp spectra in highly inhomogeneous and drifting electromagnets (25T).

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