

## Heteronuclear decoupling interference during symmetry-based homonuclear recoupling

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Recoupling methods reintroduce specific nuclear spin interactions that are normally average out by MAS, so that both the high spectral resolution afforded by MAS and the structural information provided by these nuclear spin interactions are preserved. An important set of tools to reintroduce these interactions are the symmetry-based sequences [1]. These sequences permit one to recouple selectively the interaction of interest under MAS. Particularly, two types of these sequences have been developed:  $CN_n^\square$  [2], [3], [4] and  $RN_n^\square$  sequences [2], [5].

In solid organic and biological samples, most of the applications of DQ dipolar recoupling concern  $^{13}\text{C}$  nuclei introduced by isotopic labelling. In these samples, the  $^{13}\text{C}$  nuclei experience strong  $^{13}\text{C}$ - $^{13}\text{C}$  homonuclear interactions accompanied by strong  $^1\text{H}$ - $^{13}\text{C}$  heteronuclear interactions. These  $^1\text{H}$ - $^{13}\text{C}$  heteronuclear interactions interfere with the  $^{13}\text{C}$ - $^{13}\text{C}$  homonuclear interactions, reducing the efficiency of the recoupling. This interference is suppressed normally by irradiating with a strong resonant rf field on  $^1\text{H}$  while the recoupling is performed on the  $^{13}\text{C}$  channel. However, this approach is not feasible for high MAS frequencies (around 10 kHz or more), since the required rf field on the  $^1\text{H}$  channel would be unacceptably high. This suggests that the no-decoupling regime appears at conveniently low spinning frequencies for the symmetry-based pulse sequences.

Experimental and theoretical investigation of heteronuclear interference during  $^{13}\text{C}$  homonuclear dipolar recoupling, for the case of double-quantum homonuclear recoupling pulse sequences of the symmetry class  $CN_n^\square$  and  $RN_n^\square$  is presented [6], showing that a no-decoupling regime appears for the symmetry-based pulse sequences. The effects of the spinning frequency, nutation frequency on both the  $^1\text{H}$  and  $^{13}\text{C}$  channels, and the symmetry numbers, is explored in both cases.

[1] Levitt, M. H., *Encyclopedia of Nuclear Magnetic Resonance*, 2002, 9, 165.

[2] Brinkmann, A.; Levitt, M. H., *J. Chem. Phys.*, **2001**, 115, 357.

[3] Lee Y. K.; Kurur N. D.; Helmle M.; Johannessen O.D.; Nielsen N. C.; Levitt M. H., *Chem. Phys. Lett.*, **1995**, 242, 304.

[4] Brinkmann, A.; Eden, M.; Levitt, M. H., *J. Chem. Phys.*, **2000**, 112(19), 8539.

[5] Carravetta, M.; Eden, M.; Zhao, A.; Brinkmann, A.; Levitt, M. H., *Chem. Phys. Lett.*, **2000**, 321, 205.

[6] Marin-Montesinos, I.; Brouwer, D. H.; Antonioli, A.; Wai, W. C.; Brinkmann, A.; Levitt, M. H., *J. Magn. Reson.*, **2005**, 177, 307.