Title: Measurement of transverse relaxation using spin echo methods

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Abstract:
The study of T_2 relaxation in systems with homonuclear J-coupling is complicated by modulation in the relaxation curve. This J-modulation can be removed when CPMG sequence is used and the period of repetition of refocusing pulse τ fulfils a condition

$$\tau << \frac{1}{\Delta\nu} \qquad (1)$$

where Δν is the frequency difference of coupled nuclei. However, the condition (1) cannot be in practice always fulfilled. The aim of this work was to investigate J-modulation and relaxation behaviour of homonuclear J-coupled system in various parameters of CPMG sequence. Simulations based on numerical solution of Liouville-von Neumann equation and Redfield theory were performed. Relaxation curves of CH_2 group of citrate were measured on high-resolution NMR spectrometer. It was found that the suppression of J-modulation can be achieved also for τ longer than required by the condition (1) providing that the refocusing angle in CPMG for both J-coupling partners $\theta \neq 180°$. The simulations yielded conditions for τ when J-modulation vanishes (decoupling)

$$\tau_{rec} = \frac{2k-1}{\Delta\nu}, k = 1,2,3,... \qquad (2)$$

and when it is maximal (recoupling)

$$\tau_{dec} = \frac{2k}{\Delta\nu}, k = 1,2,3,... \qquad (3)$$

The decoupling is systematically worse in strong coupling and worsening of decoupling in τ_{dec} was observed when k is increased. The simulation of relaxation showed no significant difference in T_2 from its expecting value.

Keywords: NMR, J-coupling, T_2 relaxation, CPMG, citrate