Calculating Spectral Modulations of AB Systems During PRESS Acquisitions

Schick *et al.* (1) recently reported spectral modulations of citrate (an AB system) due to changes in sequence timing parameters of double echo (PRESS) acquisitions. The statement was made that ". . .for AB systems like citrate the evolution of the density operator cannot be calculated analytically" (1). We point out that the density matrix formalism for AB spin echoes outlined by Abragam (2) may be used to calculate spectral modulations due to changes in sequence timing parameters in PRESS acquisitions.

Ignoring off-resonance effects, the eigenvalues and eigenvectors of the Hamiltonian

$$H = \delta/2 \, (i_z - i_z') + J \, \mathbf{i} \cdot \mathbf{i}', \qquad [1]$$

and those of the conjugate Hamiltonian

$$H' = -\delta/2 \, (i_z - i_z') + J \, \mathbf{i} \cdot \mathbf{i}' \qquad [2]$$

are used to evaluate $Tr\{\sigma I_+\}$; the trace of the density operator σ for the double echo sequence $90_x - \tau_1 - 180_y - \tau_2 - 180_y - t$, operating on $I_+ = i_+ + i_+'$ (2). Here, $\mathbf{i}$ and $\mathbf{i}$ are the individual spin ½ operators for the two spins, δ the chemical shift and J, the spin-spin coupling constant. Evaluation of the trace requires evaluating three nonvanishing matrix elements using standard spin ½ algebra. The result yields the transverse magnetization as a function of time, t, following the third RF pulse. This may be analytically Fourier transformed to obtain absorption, dispersion, or magnitude mode AB spectra for arbitrary J, δ, τ_1 and τ_2. The transverse magnetization after the third pulse is found to be

$$
\begin{aligned}
I_y = \; & 4p^2q^2(p+q)^2 \cos[(d-b)t + (d-b)\tau_1 + (d-b)\tau_2] \\
& + 2pq(p^2-q^2)^2 \{\cos[(d-b)t + (d-b)\tau_2 + (d-c)\tau_1] \\
& + \cos[(d-c)t + (d-b)\tau_2 + (d-b)\tau_1] - \cos[(d-b)t \\
& + (d-c)\tau_2 + (d-c)\tau_1] - \cos[(d-c)t + (d-c)\tau_2 \\
& + (d-b)\tau_1]\} + (p-q)^2(p^2-q^2)^2 \cos[(d-c)t + (d-b)\tau_2 \\
& + (d-c)\tau_1] + (p+q)^2(p^2-q^2)^2 \cos[(d-b)t + (d-c)\tau_2 \\
& + (d-b)\tau_1] + 4p^2q^2(p-q)^2 \cos[(d-c)t + (d-c)\tau_2 \\
& + (d-c)\tau_1],
\end{aligned}
\qquad [3]
$$

where $d = J/4$, $b = -J/4 + \Omega/2$, $c = -J/4 - \Omega/2$ with $\Omega = (J^2 + \delta^2)^{1/2}$. The factors p and q are given by $p = \cos\phi/2$,

$q = \sin\phi/2$ where $\tan\phi = J/\delta$. The x-magnetization I_x vanishes during readout. Spectra are generated from Eq. [3] by analytic Fourier transformation following multiplication of Eq. [3] with a line broadening factor exp$(-R_2 t)$.

Citrate spectra acquired at 7 T with hard pulse double echo sequences demonstrated τ_1- and τ_2-dependent spectral modulations that were matched exactly by the theoretical simulations (results not shown). A more stringent test of the theory was provided at 1.5 T where experimental spectra from a 100-mM solution of sodium citrate[2] dissolved in water were obtained with a General Electric 1.5 T signa scanner (General Electric Medical Systems, Milwaukee, WI). The PRESS sequence consisted of mutually orthogonal slice selective pulses with nominal 90° and 180° flip angles and 15 mm slice thicknesses. CHESS pulse water suppression was employed and 32 signal averages were acquired. Figure 1a contains 1.5 T experimental spectra (absorption mode) with τ_1 set at 17 ms and τ_2 values of 68, 75, and 88 ms, bottom to top, respectively. Figure 1b are the simulated 1.5 T spectra of citrate for these timing parameters in the PRESS sequence. The simulated spectra were calculated using $J/2\pi = 15$ Hz
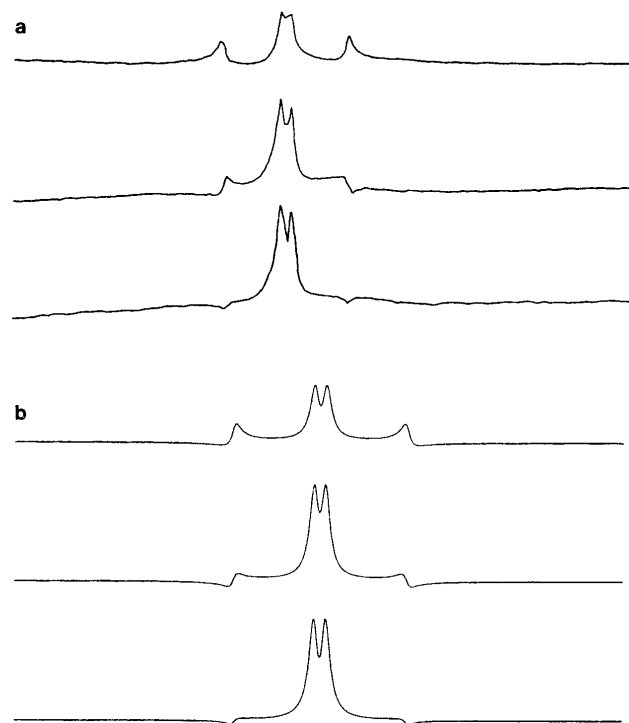

FIG. 1. (a) Experimental absorption mode PRESS spectra acquired at 1.5 T for a 100 mM citrate solution in water. The τ_1 was fixed at 16 ms and spectra were recorded with τ_2 values of 68, 75, and 88 ms, from bottom to top, respectively. (b) Theoretical absorption mode PRESS spectra for citrate at 1.5 T with the same sequence timings as in (a). There is approximately 15 Hz between adjacent inner and outer peaks.

and $\delta/2\pi = 8$ Hz and a 6-Hz line broadening factor. The theoretical spectra adequately reproduce the spectral modulations observed experimentally.

Our intent is to demonstrate that AB spectral modulations in double echo sequences are amenable to calculation. We have used a density matrix calculation based on perfect 90° and 180° pulses, though the methods can be extended to arbitrary flip angles. Even with the ideal pulse assumption, the primary spectral modulations from citrate at 1.5 T using soft pulse PRESS sequences are reproduced by the theory.

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REFERENCES

1. F. Schick, H. Bongers, S. Kutz, W.-I. Jung, M. Pfeffer, O. Lutz, *Magn. Reson. Med.* **29,** 38 (1993).
2. A. Abragam, "Principles of Nuclear Magnetism," Clarendon Press, Oxford, England, 1962.