Initial laboratory course in FYS-KJM4740

The NMR data obtained and discussed in this tutorial are acquired on a Maran Ultra NMR instrument, operating at 23 MHz proton frequency. All data are available on the home page of the course. <u>All students</u> must write up a report based on the experimental findings. Relevant raw data and model fits must be included in the report.

Exercise 1

a) The ^{1}H-NMR FID of water confined between glass beads was acquired after applying an rf-pulse for a time t_p (= 0.5, 1.0, 1.5, 2.00, 2.50, 3.0, 3.50. 4.00, 4.50 and 5.00 μs). The observed signal intensity I(t_p) is found on the home page of the course: *Exp1/Results I(t_p).* Discuss the results and calculate the strength B_1 (gauss) of the rf-pulse?

b) The ^{1}H-NMR FID (real/imaginary) of water confined between glass beads was acquired with an apparent rf-offset denoted O1. The results are found on the home page of the course: *O1 nnnnnn.0001.Dat.*
It is known that the actual frequency offset Δν (or the frequency in the rotating frame of reference) is related to O1 by the formula:

$$\Delta\nu = \nu_{rf} - \nu_0 = O1 + \text{constant (Hz)} \qquad (1)$$

With ν_0 being the Larmor frequency of the nucleus and ν_{rf} is the frequency of the radio pulse. Hence, the real part *R(t)* of the FID reads:

$$R(t) = I_0 \cos(2\pi\Delta\upsilon \cdot t + \theta) \qquad (2)$$

where θ represents the phase shift. Determine the period length P (in seconds) from the real part *R(t)* of the FID and calculate:

$$\Delta\nu = 1/P \qquad (3)$$

for each O1. Plot Δν (Eq 3) against O1 and discuss your results. Are your results in agreement with Eq 1?

c) The FID is acquired on-resonance. For a liquid, the FID or F(t) is theoretically expected to be described by a single exponential function. Hence, fit F(t) to a single exponential function: $\exp(-R_2 t)$ as well as to a single Gaussian function: $\exp(-(R_2' t)^2)$ and try to explain your results
(Hint: inhomogeneous magnetic field).

d) A 90^0 rf-pulse followed by a repetition delay time t_{RD} and a subsequent 90^0 rf-pulse (measuring pulse) is applied on water confined between glass beads for four (4) different repetition delays t_{RD} (= 3s, 2s, 1s and 0.5s). The observed FID is denoted F(t; t_{RD}) with t being time. Show that:

$$F(0,t_{RD}) = F(0,\infty)\left[1-\exp(-t_{RD}/T_1)\right] = F_0\left[1-\exp(-t_{RD}/T_1)\right] \quad (4)$$

where F($0;t_{RD}$) represents the signal intensity at t = 0 for a given delay time t_{RD}. Measure F($0;t_{RD}$) (File: Exp1/RD ns) for all t_{RD} and determine F_0 and T_1 from Eq 4 by model fitting.

Exercise 2

Inversion Recovery experiments are performed on a series of CuSO4-solutions (concentration C = 20mM, 10mM, 5mM, 2.5mM, 1.25mM and 0mM). The data are available on the homepage of the course, file: *Exp2/nn mM-CuSO4-T1*.
Show that:

$$F(\tau) = F_0\left[1-\alpha\cdot\exp(-\tau/T_1)\right] \quad (5)$$

Where F_0 is the equilibrium magnetization ($F_0 \approx F(\tau = 5T_1)$) and α equals 2.00. The experimental parameter τ represents the time between the initial 180^0-rf pulse and the subsequent 90^0 rf-pulse (measuring pulse). Determine T_1 by model fitting Eq 5 to the observed relaxation data. Use α as an adjustable parameter.
Plot the spin-lattice relaxation rate R_1 (= $1/T_1$) as a function of the CuSO4 concentration $C(CuSO_4)$. Present all data/fits in one Figure and discuss your results.

Exercise 3

CPMG experiments are performed on a series of CuSO4-solutions (concentration C = 20mM, 10mM, 5mM, 2.5mM, 1.25mM and 0mM) and the data are available on the homepage of the course, file: Exp3/CPMG nn MM. It is known that the signal intensity of the CPMG envelope can be written:

$$I(2\tau) = I_0\cdot\exp(-2\tau/T_2) \quad (5)$$

where I_0 is the equilibrium magnetization and T_2 defines the spin-spin relaxation time. Determine T_2 by model fitting Eq 5 to the observed relaxation data. Plot the spin-spin relaxation rate R_2 (= $1/T_2$) against $C(CuSO_4)$. Show all data/fits in one Figure and discuss your results.