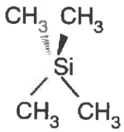
S-66.3320 NMR perusteet **Tentti 9.3.2015**

Suorita 5 tehtävää tehtävistä 1-6! Laskimen muistiin ei saa olla talletettu kirjoitettua informaatiota. Tehtäväpaperin lopussa on apuvälineitä tenttiä varten.

1. a) If I is the angular momentum quantum number, what is the length of the angular momentum vector? (1,5p) **b)** Which of the following statements **i)**, **ii)** and **iii)** must be correct, which might possibly be correct, and which cannot be correct? Give reasons! **i)** The nucleus ^{89}Y (atomic number = 39) has a ground state spin I = ½. **ii)** The nucleus ^{90}Zr (atomic number = 40) has a ground state spin I = 1. **iii)** The nucleus ^{91}Zr (atomic number = 40) has a ground state spin I = ½. (3p) **c)** If a particle with spin S = 3/2 couples to a particle with spin S = 1/2, what are the possible values for the spin of the resulting particle? (1,5p)

2. Consider a chemical compound and its NMR spectrum. Suppose that a sample is a tube containing pure liquid tetramethylsilane , $Si(CH_3)_4$ (TMS). The molecular structure is shown in the figure below.

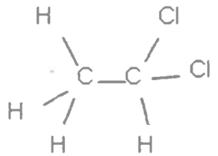


The isotopes are in Table below.

Isotope	Spin	Natural abundance/%	$\gamma/10^6$ rad s^{-1} T^{-1}
^{1}H	1/2	~ 100	267.5
^{12}C	0	~ 98.9	–
^{13}C	1/2	~ 1.1	67.3
^{28}Si	0	~ 92.2	–
^{29}Si	1/2	~ 4.7	–53.2
^{30}Si	0	~ 3.1	–

a) Calculate the relative proportion of isotopomer $^{28}Si(^{12}C^1H_3)_3\,(^{13}C^1H^3)$ in the sample using the abundances of the table! (3p) **b)** The magnetic field is 9.3950T . Calculate the larmor frequencies of the spins ^{28}Si, ^{12}C, and ^{1}H! Sketch the NMR spectrum of the isotopomer $^{28}Si(^{12}C^1H_3)_3\,(^{13}C^1H_3)$! (3p)

3. Describe the ^{1}H and ^{13}C spectra of the compound below. Assume isotopic abundances of 100% for ^{1}H and 1% for ^{13}C. Assume that the one-bond ^{13}C-^{1}H J-couplings are around 135 Hz and the three-bond ^{1}H-^{1}H J-couplings are 7 Hz. Ignore the couplings to the Cl nuclei. In your answer, describe which multiplets are there in the ^{1}H and ^{13}C spectra! Give reasons for the multiplets! (6p)



4. Consider a x-pulse which transfers spin population in an inversion state by rotating it around suitable axis. **a)** What is the density matrix of the system before the pulse? (2p) **b)** How does the density matrix change during this pulse? (4p) (Hint: Assume that the spins are initially in equilibrium with the external magnetic field in temperature T. In thermal equilibrium the population ratio obeys Boltzmann equation.)

5. a) Explain the pulse sequence of figure 5.1. (2p) **b)** Explain the change in the spin density matrix in different intervals and explain the signal $a(\tau)$ of figure 5.2. (4p)

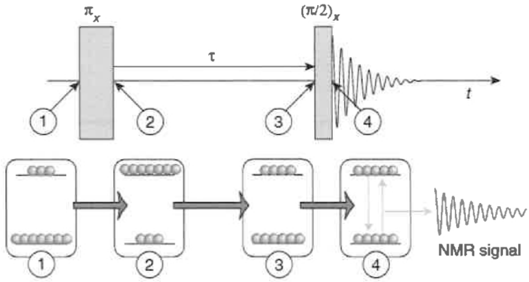


Figure 5.1

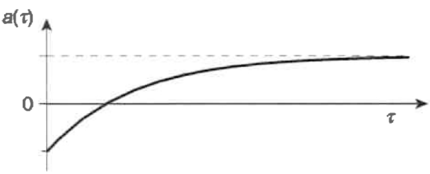
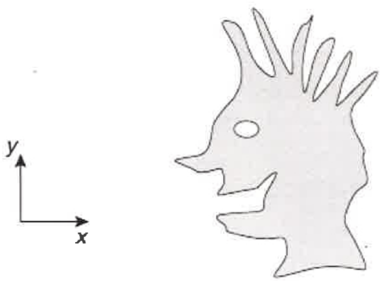


Figure 5.2

6. We wish to make an image of two dimensional object figure below. **a)** Draw a NMR imaging pulse sequence for this task! (2p) **b)** Give the larmor frequencies in different parts of the sequence! (1p) **c)** Give the nutation frequencies in detail and the components of the spin matrix in different parts of the sequence. Give also the formulas! (3p)



Alla apuvälineitä tenttiä varten!

Angular momentum operators in the Zeeman eigenbasis $\{|\alpha\rangle|\beta\rangle\}$

$$\hat{I}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{I}_y = \frac{1}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \hat{I}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin-1/2 rotation operators

$$\widehat{R}_x(\beta) = \begin{pmatrix} \cos\frac{1}{2}\beta & -i\sin\frac{1}{2}\beta \\ -i\sin\frac{1}{2}\beta & \cos\frac{1}{2}\beta \end{pmatrix}$$

$$\widehat{R}_y(\beta) = \begin{pmatrix} \cos\frac{1}{2}\beta & -\sin\frac{1}{2}\beta \\ \sin\frac{1}{2}\beta & \cos\frac{1}{2}\beta \end{pmatrix}$$

$$\widehat{R}_z(\beta) = \begin{pmatrix} \exp\{-i\frac{1}{2}\beta\} & 0 \\ 0 & \exp\{+i\frac{1}{2}\beta\} \end{pmatrix}$$

Gyromagnetic ratio of ^1H is 267.522 x 10^6 rad s^{-1} T^{-1}
Planck's constant h is $6.62606957 \times 10^{-34}$ Js