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Department of Chemistry

# Examination paper for KJ3021 – NMR

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**Problem 1.**

Which processes are responsible for the NOE effect?

a) single-quantum relaxation processes
b) zero-quantum relaxation processes
c) double-quantum relaxation processes
d) quadrupolar relaxation processes
e) non-dipolar relaxation processes
f) polarization transfer

(4 p)

**Problem 2.**

Which are the two main reasons for using deuterated solvents in NMR?

(4 p)

**Problem 3.**

What is the purpose of using Fourier transformation in NMR?

a) to improve spectra appearance

b) to make spectra of the same compound appear identical, independently on which instrument (field strength) is used

c) to enhance resolution and signal intensity

d) to get a spectrum from the free induction decay

(2 p)

**Problem 4**

Describe a proton experiment with water suppression, based on a difference in T1 relaxation time constants between water and a sample (small organic molecule).

(10 p)

**Problem 5**

Mark the correct statements:

a) HMQC is phase sensitive, allowing for distinction of $CH/CH_3$ from $CH_2$ groups.

b) COSY45 is used when difference in chemical shifts between coupling protons is large.

c) COSY experiment can be optimized for long range H,H couplings.

d) 2D NOESY experiment can be used for middle size molecules.

e) an ordinary HMBC experiment cannot be phased.

f) edited HSQC spectrum cannot be phased, because it gives signals in magnitude mode.

(4 p)

**Problem 6.**

1D and 2D NMR spectra (500 MHz, $CDCl_3$) of an unknown compound are available on the link below. It is a hydrocarbon, whose molecular formula can be found from $^{1}H$ and $^{13}C$ spectra. Elucidate the structure and assign all $^{1}H$ and $^{13}C$ shifts.

(30 p)

**Problem 7.**

Structure of the compound is shown on Fig. 1 and its 1D and 2D NMR spectra are available on the link below. ***Note that signal at 144.9 ppm in 1D $^{13}C$ spectrum is of very low intensity***.

Assign all $^{1}H$ and $^{13}C$ resonances. Make a table as shown below and fill in the shifts according to the enumeration given on the structure.

(21 pts)

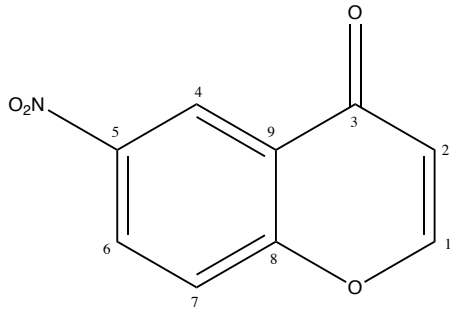


Figure 1.

| Carbon no. | δ $^{13}C$ (ppm) | δ $^{1}H$ (ppm) |
|---|---|---|
| 1 | | |
| 2 | | |
| 3 | | |
| 4 | | |
| 5 | | |
| 6 | | |
| 7 | | |
| 8 | | |
| 9 | | |

**Problem 8.**

Structure of the compound is shown on Fig. 2 and its 1D and 2D NMR spectra are available on the link below. Assign all $^{1}H$ and $^{13}C$ resonances. Make a table as shown below and fill in the shifts according to the enumeration given on the structure.

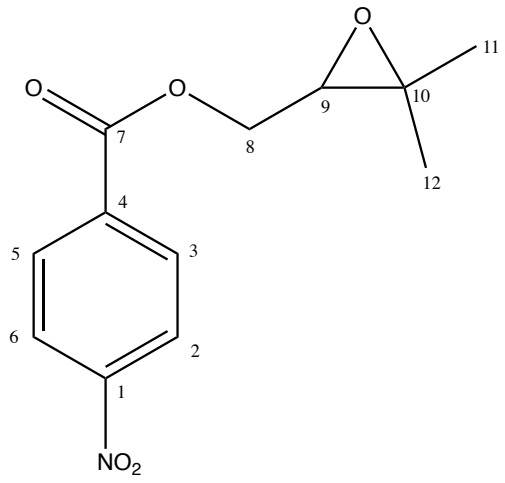


Figure 2.

| Carbon no. | δ $^{13}$C (ppm) | δ $^{1}$H (ppm) |
|---|---|---|
| 1 | | |
| 2 | | |
| 3 | | |
| 4 | | |
| 5 | | |
| 6 | | |
| 7 | | |
| 8 | | |
| 9 | | |
| 10 | | |
| 11 | | |
| 12 | | |

(25 pts)