Model answer
Part II

Answer the following questions:

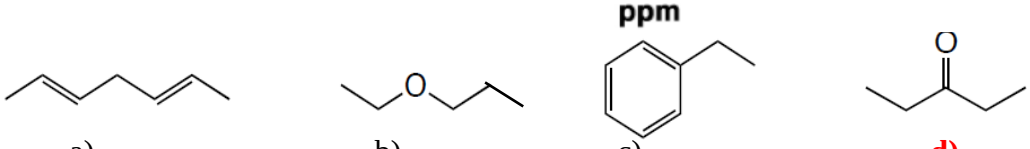
1- Choose the correct answer: (20 Marks)

1. How many signals would you expect to find in the ^{1}H NMR spectrum of $CH_3OCH_2OCH_3$?
   a) 1 **b) 2** c) 3 d) 4

2. The structure for a compound, $C_4H_8Br_2$, which has the following proton NMR spectrum Doublet δ 1.7 (6 H) and Quartet δ 4.4 (2 H) is:
   a) 1,1-dibromobutane **b) 2,3-dibromobutane** c) 1,3-dibromobutane d) 1,2-dibromobutane

3. The chemical shift of the signal has been reported at 900 Hz downfield from TMS in an NMR spectrometer with a 450-MHz operating frequency is:
   a) 0.5 **b) 2** c) 8 d) 4

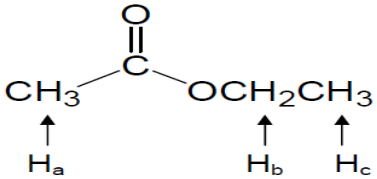
4. What is the most likely structure of the molecule that gave the following ^{1}H NMR spectrum?



a) b) c) **d)**

5. A triplet and quartet pattern in ^{1}H NMR often indicates the presence of a (an):
   a) phenyl group b) isopropyl group c) propyl group **d) ethyl group**

6. Arrange the indicated protons in the following molecule in order of increasingly downfield chemical shift?

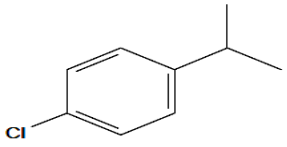


a) $H_c < H_b < H_a$ b) $H_a < H_b < H_c$ c) $H_b < H_a < H_c$ **d) $H_c < H_a < H_b$**

7. Which of the following nucleus cannot be detected by nuclear magnetic resonance spectroscopy?
   a) $_6C^{12}$ b) $_6C^{13}$ c) $_9F^{19}$ d) $_1H^2$

8. How many sets of equivalent protons are there for $CH_2Cl–CH_2$ - CH_2 Cl
   a) 2 b) 1 c) 3 d) 4

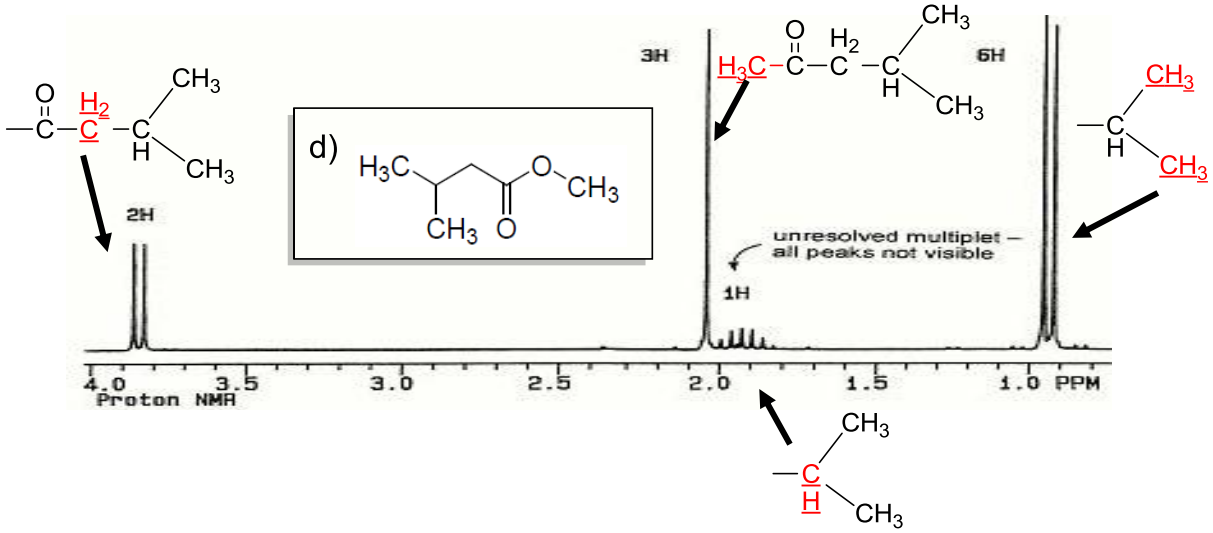
9. For the compound below, how many signals (peaks) would you expect in its ^{1}H NMR spectrum?



a) 4 b) 5 c) 6 d) 7

10. What is the degree of unsaturation of a compound with formula $C_3H_6O_2$?
    a) 1 b) 2 c) 3 d) 0

2- a) - Match the spectrum to one of the compounds shown below. Justify your answer by assigning the peaks to the protons in the structure you have chosen. (5 Marks)



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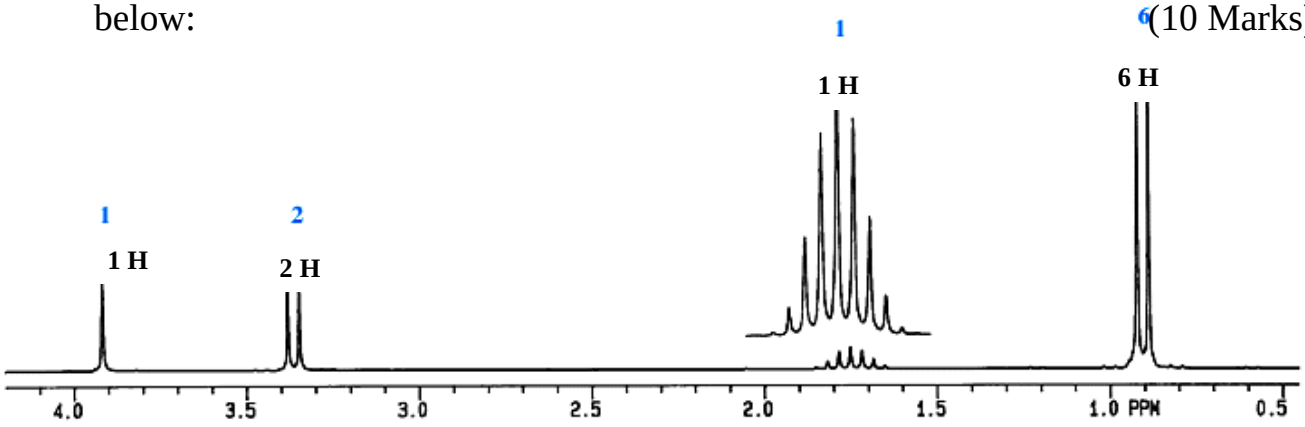
b) Deduce the structure of an organic compound with the molar mass 74 g/mol has the composition 64.86% of C and 13.51% of H. Its ^{1}H NMR spectra shown below: (10 Marks)



O % = 100 – (64.86+13.51) = 21.63

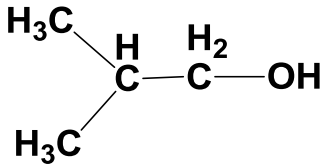
C	H	O
64.86/12	13.51/1	21.63/16
٥.٤٠٥/١.٣٥١	١٣.٥١/١.٣٥١	١.٣٥١/١.٣٥١
٤.٠٠	١٠.٠٠	١.٠٠

I.F = $C_4H_{10}O$ = M.F

	a	b	c	d
δ(ppm)	٠.٩	١.٧	3.35	٣.٩
Mult.	d	m	d	s
Ratio	6	١	2	1
No. of protons	6	١	2	1
Gorups	2(-CH_3)	CH	-CH2	OH

I.H.D = 2*4 +2 – 10 / 2 = 0 This compound is saturated

The structure is



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c) Explain the following factors influencing on chemical shift: (5 Marks)

i- Electroinc effect.

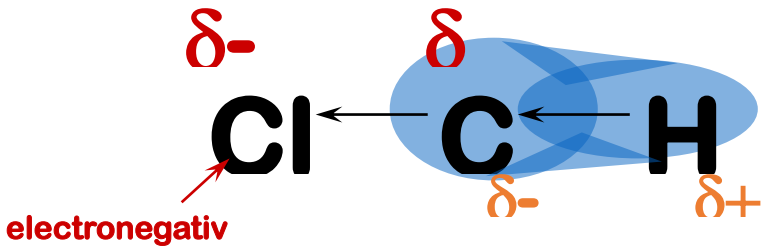
ii- Hydrogen bond.

Answer

i- Electroinc effect.

1- Electronegativity Effects:

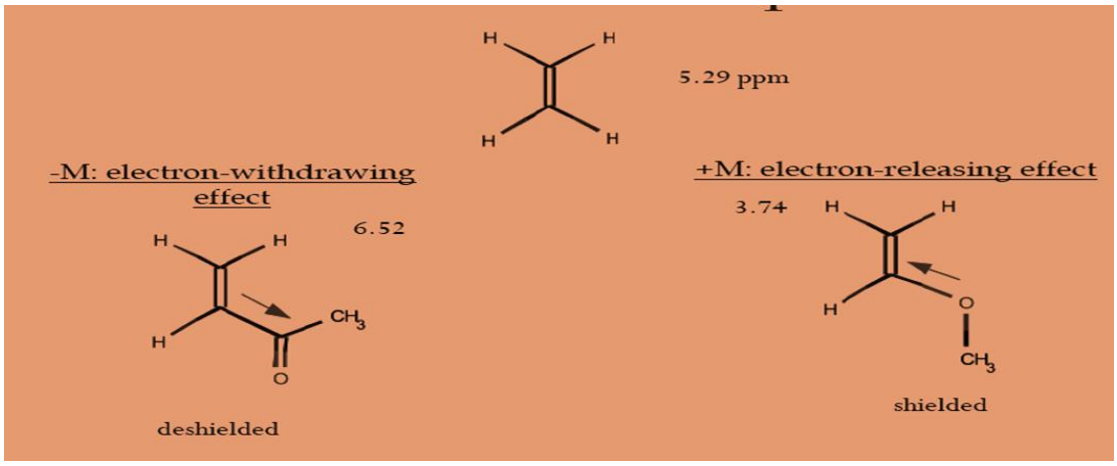
Electronegative elements directly attached to a carbon atom bearing hydrogens (protons) pull electron density away from the protons. These protons are **deshielded** "



Chlorine "deshields" the proton, that is, it takes valence electron density away from carbon, which in turn takes more density from hydrogen deshielding the proton.

1- Mesomeric Effects

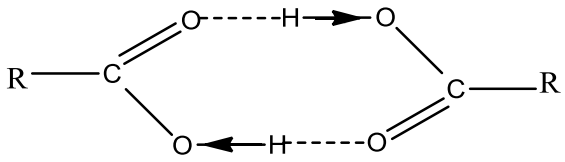
The mesomericeffector resonance effect in chemistry is a property of the substituents or functional groups in a chemical compound. The mesomeric effect is negative (-M) when the substituent is an electron-withdrawing group and the effect is positive (+M) when based on resonance the substituent is an electron releasing group.



ii- Hydrogen bond.

Hydrogen Bonding Effects:

Hydrogen bonding causes a further deshielding of protons, and a further downfield shift for these proton resonances. Hydrogen bonding effects are concentration and temperature dependent, and this results in a wide range of possible resonance frequencies for these protons. In general, protons attached to oxygen and nitrogen resonate between 0.5 - 5 ppm.



- Resonance, electronegativity of oxygen and the formation of hydrogen bonding withdraw electron cloud from the acid protons.
- Thus, protons attached to carboxylic acids are the least shielded protons and have a chemical shift of 10-12 ppm.