

M. SC. (Organic Chemistry) Sem-III (Choice Based Credit & Grade System) : WINTER - 2018

SUBJECT : SPECTROSCOPIC METHODS IN STRUCTURE DETERMINATION

Day : Monday
Date : 22/10/2018

W-2018-0992

Time : 03.00 PM TO 06.00 PM
Max. Marks : 60

N.B.:

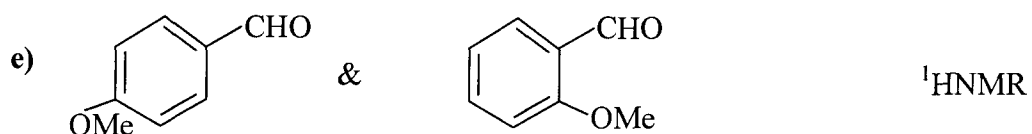
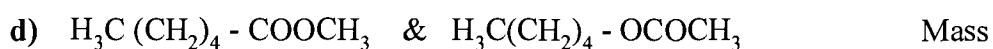
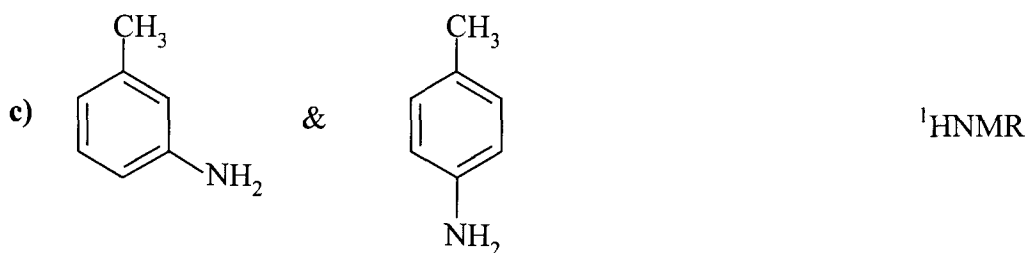
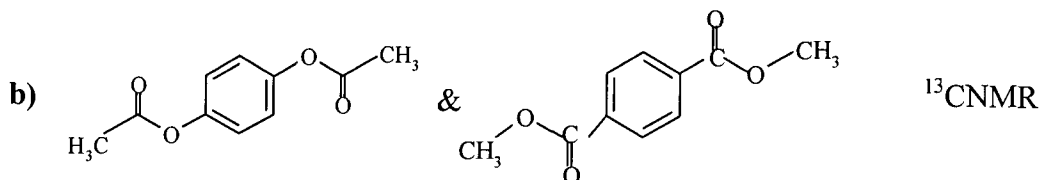
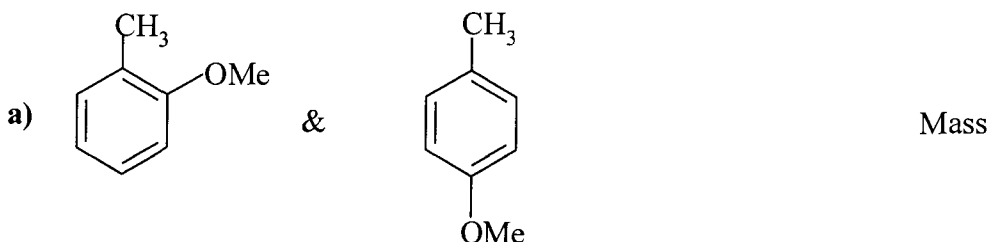
- 1) All questions are **COMPULSORY**.
- 2) Figures to the right indicate **FULL** marks.
- 3) Answers to both the sections should be written in the **SEPARATE** answer books.

SECTION – I

Q.1 Explain ANY THREE of the following: [15]

- a) In the PND spectrum coupling information is lost.
- b) Spin states of methylene protons in ethyl alcohol, affect the lines obtained for methyl protons.
- c) Quaternary carbons in ^{13}C NMR shows weak intensity signals.
- d) CH_2DBr shows a triplet with 1:1:1 intensity ratio in PMR.
- e) Methyl – n – butyrate gives strong peak at m/e 74.

Q.2 Distinguish between ANY THREE of the following by given spectral method: [15]



P.T.O.

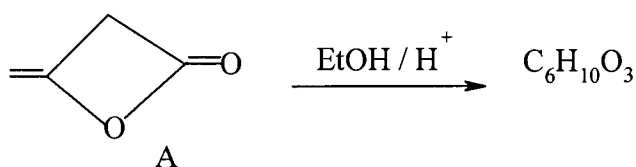
SECTION – II

Q.3 Write short notes on **ANY THREE** of the following: [15]

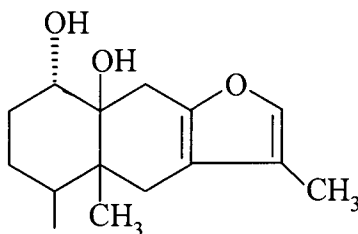
- a) Karplus equation
- b) Working of single and double focusing Mass Spectrometer
- c) Two methods for simplifying complex ^1H NMR spectrum
- d) Off resonance spectroscopy
- e) Spin decoupling

Q.4 Attempt **ANY THREE** of the following: [15]

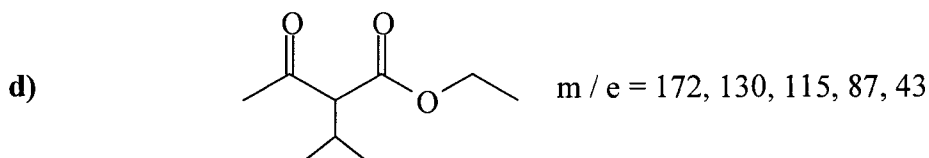
- a) In an AMX spectrum chemical shifts of A, M and X protons are 2.3, 3.5 and 6.46 δ . $J_{AM} = 7$ Hz, $J_{AX} = 11$ Hz and $J_{MX} = 5$ Hz. Calculate the line positions of all lines at 100 MHz spectrometer. Explain your answer.
- b) Compound A in the following reaction gives a product having molecular formula $\text{C}_6\text{H}_{10}\text{O}_3$. The product shows following data:
 IR : 1745, 1710 cm^{-1}
 ^1H NMR : 1.28 (t, $J = 7$ Hz, 3H); 2.21 (s, 3H);
 3.24 (s, 2H); 4.2 (q, $J = 7$ Hz, 2H)
 ^{13}C NMR : 203, 170, 62, 39, 22, 17.
 Deduce the structure and justify.



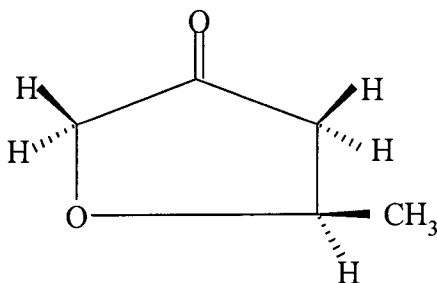
- c) Assign the CMR signals given below to different carbons in the following compound. Justify your answer.



Signals at : 80(q), 17.0 (q), 20 (q), 28 (t), 29 (t), 34(t), 35(t), 49(s), 72(d), 82(d), 85(s), 125(s), 128(s), 135(d), 148(s).



- e) ^1H NMR spectrum of the given compound shows the following signals. Assign the chemical shift and comment on coupling constant.



1.42 (d, $J = 6$ Hz, 3H), 1.80 to 2.90 (m, 2H)
 3.83 (d, $J = 16.5$ Hz, 1H), 4.04 (d, $J = 16.5$ Hz, 1H), 4.35(d of quintet, 1H).

* * * *