

**M. SC. (ORGANIC CHEMISTRY) SEM-III (CHOICE BASED
CREDIT & GRADE SYSTEM) : SUMMER - 2018**
SUBJECT : SPECTROSCOPIC METHODS IN STRUCTURE DETERMINATION

Day : **Monday**
Date : **23/04/2018**

S-2018-0879

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

N.B.:

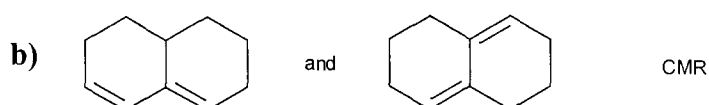
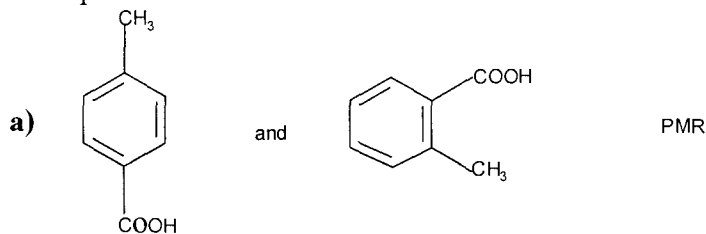
- 1) All questions are **COMPULSORY**.
- 2) Figures to the right indicate **FULL** marks.
- 3) Answers to both the sections should be written in **SEPARATE** answer books.

SECTION – I

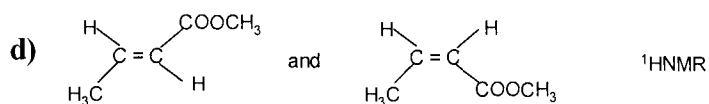
Q.1 Explain **ANY THREE** of the following: **[15]**

- a) CH_2F_2 shows a triplet in PMR.
- b) The – OH proton usually appears at a lower field in DMSO than in CDCl_3 .
- c) How chemical ionization method is used in mass spectrometry?
- d) $\text{DMSO} - d_6$ shows seven lines in $^1\text{HNMR}$.
- e) Signal intensities of CMR are very weak as compared to PMR.

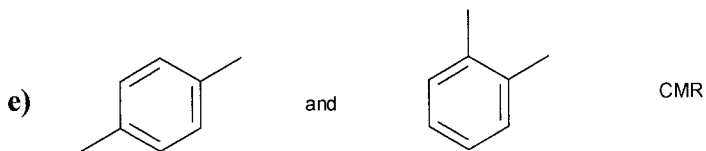
Q.2 Distinguish between **ANY THREE** of the following pairs using the given **[15]** spectral method:



c) $\text{H}_3\text{C}(\text{CH}_2)_4\text{CHO}$ and $\text{H}_3\text{CCH}_2\text{COCH}_2\text{CH}_2\text{CH}_3$ (Mass)



P.T.O.



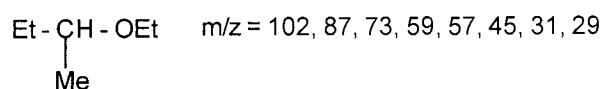
SECTION – II

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

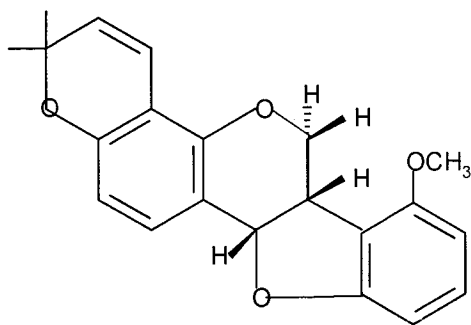
- COSY
- Shift reagents
- Chemical exchange reaction
- Metastable ions
- DEPT

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

- Explain the genesis of the following:



- Identify the structures of the following compounds from the CMR spectra:
 - MF : C₈ H₈ O : 50.8 (t), 52.1 (d), 125.4 (d, strong), 128 (d), 128.4 (d, strong), 137 (s, weak)
 - MF : C₉ H₁₂ : 21.2 (q), 127.2 (d), 137.5 (s)
- Assign the signals to the various protons in the structure. Justify your answer.



1.42 (s, 6H), 3.69 (m, 1H), 3.76 (m, 1H), 3.85 (s, 3H), 4.33 (m, 1H)
 5.45 (d, J = 7Hz, 1H), 5.56 (d, J = 10Hz, 1H), 6.45 (dd, J = 8 and 2Hz, 1H)
 6.50 (dd, 8 and 2Hz, 1H), 6.53 (d, J = 9Hz, 1H), 6.67 (d, J = 10Hz, 1H),
 7.05 (d, J = 9Hz, 1H), 7.12 δ (t, J = 8Hz, 1H)

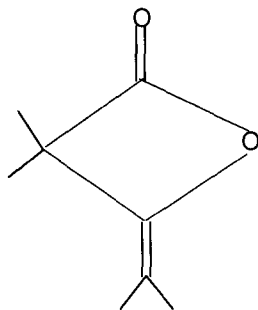
...3...

d) Deduce the structure based on the following data:

i) Molecular formula : $C_4H_8O_2$
CMR : 92.8 (t),
: 65.9 (t, strong)
: 26.6 (t)

ii) Molecular formula : C_5H_8
IR : 1640 cm^{-1}
PMR : 1.92 δ (quintet, 5Hz, 2H)
: 2.7 δ (dt, 5 and 6Hz, 4H)
: 4.7 δ (t, 6Hz, 2H)

e) The following compound showed signals in ^1H NMR and ^{13}C NMR Spectrum.
Assign the signals for protons and carbons:



$\delta = 173$ (s), 146 (s), 103 (s), 54 (s), 20 (strong, q), 16 (q), 15 (q)
 $\delta = 1.44$ (s, 2H), 1.54 (s, 3H), 1.65 (s, 3H), 1.68 (s, 3H)

* * * *