

**M.Sc. DEGREE III SEMESTER EXAMINATION IN APPLIED CHEMISTRY
NOVEMBER 2012**

CHE 2312 SPECTROSCOPY - B

Time : 1½ Hours

Maximum Marks : 25

PART A

(2 x 5 = 10)

- I. 1. An organic compound of molecular formula $C_{10}H_{12}O_3$ gave an electron impact mass spectrum whose peaks are given below:

m/e	Relative Intensity
77	12.9
107	100
135	41
180	37.5

The 1H NMR spectral data in δ (ppm) of this compound are:

1.39 (3H,t(J=7Hz)), 3.56 (2H,s), 3.98 (2H,q(J=7Hz)), 6.83 (2H,d(J=8Hz)),
7.18 (2H,d(J=7Hz)), 12.5 (1H,bs).

The normal C-13 and the DEPT-135 and DEPT-90 data of the compound are:

Normal carbon 15 ppm	DEPT-135	DEPT-90
15 ppm	Positive	No peak
40	Negative	No peak
63	Negative	No peak
115	Positive	Positive
125	No peak	No peak
130	Positive	Positive
158	No peak	No peak
179	No peak	No peak

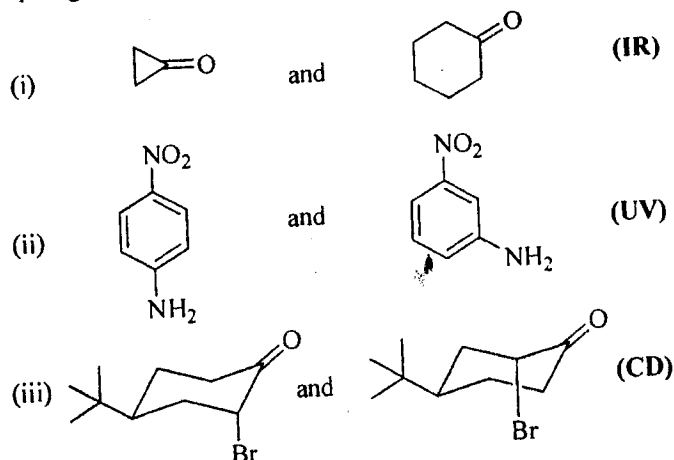
Deduce the structure of the compound in agreement with the above data.

2. A compound with molecular weight 120 showed negative to iodoform test. In UV, it absorbs at $292 \text{ m}\mu$ $\epsilon_{\text{max}} 16$. In the IR spectrum, the important bands of the compounds are: 3042 (m), 2941 (w), 2862 (w), 1722 (s), 1605, 1575 (m) and 1462 (m) cm^{-1} . The 1H NMR signals in δ (ppm) of the compound are: 7.27 (26.5 squares, multiplet), 2.8 (10.3 squares, doublet), 0.88 (5.2 squares, triplet). Deduce the most probable structure of the compound consistent with the above data.

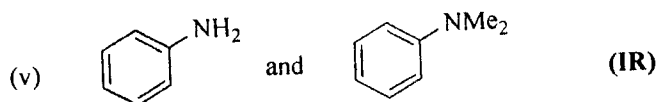
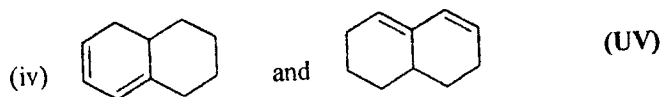
PART B

(3 x 5 = 15)

- II. A How will you distinguish each of the following pairs of compounds using the techniques given in the parenthesis? (5)



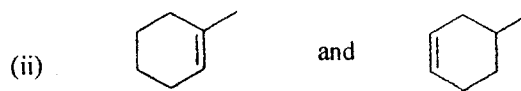
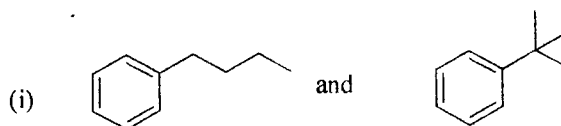
(P.T.O)



OR

- B (a) How will you distinguish inter- and intramolecular H-bonding using spectroscopic techniques? Explain with examples. (3)
 (b) Discuss the utility ORD in the study of stereochemistry of organic compounds with example. (2)

- III. A (a) How will you distinguish each of the following pairs of compounds using mass spectra? (3)

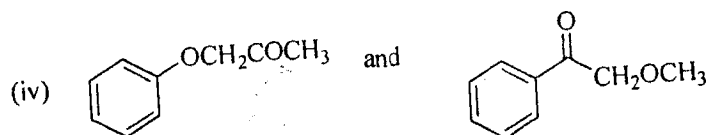
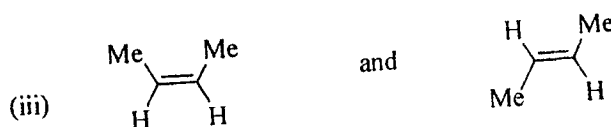
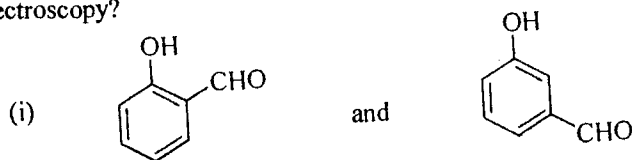


- (b) Based on the mass spectral data, suggest the fragmentation pattern for each of the compounds given below: (2)
 (i) *p*-Aminoethylbenzene: m/z 165, 137, 120, 92
 (ii) *Benzyl methyl ketone*: m/z 134, 119, 92, 91, 65, 57, 43

OR

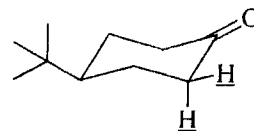
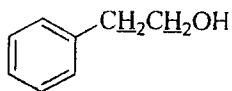
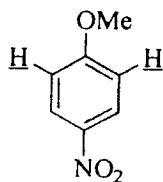
- B (a) Explain metastable ions and their usefulness in figuring out fragmentation patterns. (2)
 (b) Briefly discuss the theory and instrumentation of tandem mass spectrometry and its advantages over the other methods. (3)

- IV. A (a) How will you distinguish each of the following pairs of compounds using NMR spectroscopy? (2)



(Continued.....3)

- (b) (i) Define 'magnetic equivalence' (1)
 (ii) Indicate whether the underline protons in each of the molecules shown below are magnetically equivalent. Give your reasoning. (2)



OR

- IV. B (a) Discuss briefly the theory and application of NOE in structural elucidation of organic compounds. (3)
 (b) Briefly outline the importance of correlation spectroscopy with examples in structural elucidation. (2)
