DEPARTMENT OF SCIENCES, M. Sc. (C)
II SEMESTER END SEMESTER EXAMINATIONS, APRIL 2017

SUBJECT: ORGANIC SPECTROSCOPY – II [CHM 608]
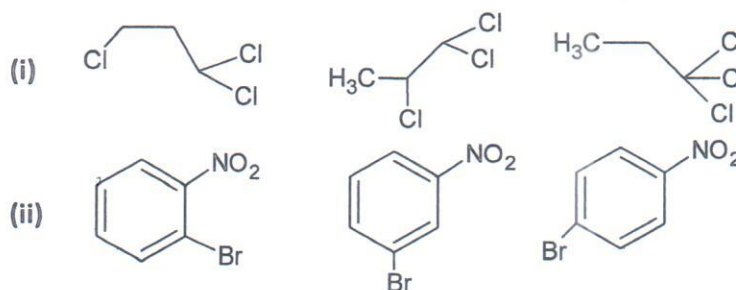**(REVISED CREDIT SYSTEM)**

Time: 3 Hours   Date: 27th April, 2017   MAX. MARKS: 50
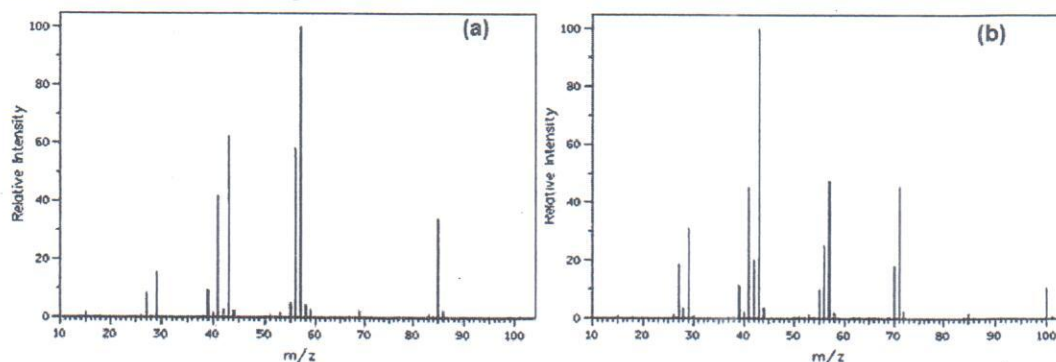
Note: Answer **any five full** questions.

1.A.   What are soft ionization techniques? Discuss any three of them.

1.B.   Explain, how the following compounds can be differentiated by ^1H NMR spectroscopy?

(i)

(ii)

1.C.   Find the mass spectrum corresponding to heptane and 2,2,3-trimethylbutane from the following spectra and explain it.

[4+4+2]

2.A.   (i)   Explain, why the splitting of signals are not due to C – C coupling in ^{13}C NMR spectroscopy?

(ii)   Give reason: Benzene anion is an ESR active whereas benzene is not.

2.B.   (i)   The spin of ^{59}Co is 7/2. Assuming an axial field gradient, obtain expressions for frequencies of the NQR transitions.

(ii)   Explain the expected ESR spectrum of 4-nitrobenzoate dianion.

2.C.   Why the source and absorber in Mossbauer spectroscopy are bound in crystal lattices and are cooled to low temperatures?

[4+4+2]

3.A. Define chemical shift. Explain how anisotropic effect affect the chemical shift values in case of ethene, ethyne and benzene.

3.B. Discuss the following:
   (i) Ion Cyclotron resonance mass spectrometry
   (ii) Chemical shift reagents

3.C. (i) The hydroxyl protons of an alcohol have variable chemical shift values in ^1H NMR spectrum. How to confirm the presence of O-H group in the structure?
   (ii) Explain the number of peaks and their splitting pattern of ^1H NMR spectrum of CH_2ClCH_2Cl.

[4+4+2]

4.A. Explain the theory of ESR spectroscopy.

4.B. Predict and explain the Off-resonance and DEPT – NMR spectra of the following compounds
   (i) 1,2,2-trichloro propane   (ii) 4-ethoxy benzaldehyde

4.C. Calculate the recoil velocity of a Mossbauer nucleus of ^{57}Fe when emitting a γ-ray of energy 14.4 keV. If the mass is changed to 100 g/mol, what will be the recoil velocity? Given: 1eV = 1.6×10^{-19} J.

[4+4+2]

5.A. Explain the principle involved in HPLC-MS technique. Discuss the various designs of interfaces between HPLC-MS and GC-MS.

5.B. (i) The mass spectral data of an unknown liquid are given below. What is the molecular formula of this unknown?

m/z	Intensity (mm)
112	53
113	3.8
114	0.5

   (ii) Explain with an example, the Retro Diels-Alder fragmentation.

5.C. Give reasons for the following;
   (i) Strong molecular ion peak is observed in case of aromatic hydrocarbons with no long side chains.
   (ii) The increase in temperature or dilution affects the resonance position of OH proton in NMR spectra of p-nitro phenol.

[4+4+2]

6.A. Discuss the applications of NQR spectroscopy.

6.B. Predict the ^{13}C chemical shift values for various carbons of the following molecules;
   (i) n-Pentane
   (ii) 3-Pentamine (correction for internal NH_2: α carbon = +24, β carbon = +10, γ carbon = − 5)
   (iii) Nitrobenzene (correction for NO_2: C1 = + 19.6, C2 = − 5.3, C3 = + 0.9, C4 = + 6.0)
   (iv) 1-Fluoro-2-Nitrobenzene (correction for NO_2: C1 = + 19.6, C2 = −5.3, C3 = + 0.9, C4 = + 6.0) (correction for F: C1 = + 35.1, C2 = −14.3, C3 = + 0.9, C4 = − 4.5)

6.C. Differentiate between ESR and NMR spectroscopic techniques.

[4+4+2]

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