MANIPAL
ACADEMY of HIGHER EDUCATION
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Reg. No.

DEPARTMENT OF SCIENCES, III SEMESTER M.Sc (Chemistry)
END SEMESTER EXAMINATIONS, DEC. 2020
SPECTROSCOPY – II [CHM 5101]

(REVISED CREDIT SYSTEM-2017)

Time: 3 Hours Date: 29 Dec 2020 MAX. MARKS: 50

Note: (i) Answer **ALL** questions.
(ii) Draw diagrams, and write equations wherever necessary

1.A. Explain the instrumentation of Laser ionization of mass spectrometry. Differentiate between hard and soft ionization techniques.

1.B. What is non first order spectra? Discuss about three methods used to resolve non first order spectra

1.C. Illustrate with appropriate examples, the application of isotope substitution in mass spectrometric analysis of samples.

(4+4+2)

2.A. Explain the expected broad band proton decoupled and the off-resonance spectra of 1,2,2-trichloro propane.

2.B. Deduce the expressions for frequencies of NQR transitions of an axially symmetric system with a spin (I) of 5/2.

2.C. Estimate the ^{13}C chemical shift (δ) values of unsaturated carbons in (*Z*)-3-methyl-2-pentene (correction for Z-cis is -1.1).

(4+4+2)

3.A. **i)** Discuss about the signals expected in the ^{1}H NMR spectra of methyl butanoate and ethyl propanoate.

ii) Give reasons for the following;

a) Base peak is not the molecular ion peak in case of compounds like benzyl chloride

b) The increase in dilution affects the resonance position of OH proton in NMR spectra of p-nitro phenol.

3.B. Describe the Mössbauer spectrometer and its working with a neat diagram.

3.C. Explain the principle involved in GC-IR-MS.

(4+4+2)

4.A. **(i)** Write briefly about the COSY and DEPT of nuclear magnetic resonance spectroscopic techniques.

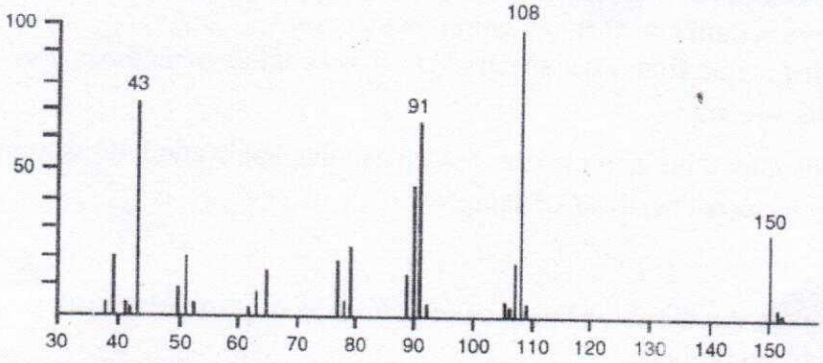
(ii) A free Mossbauer nucleus, ^{57}Fe makes a transition from the excited state of energy 14.4 keV relative to its ground state. Calculate the recoil energy of the nucleus. Given: 1 eV = 1.6×10^{-19} J, $h = 6.626\times10^{-34}$J.s

4.B. Discuss the factors affecting the ^{13}C chemical shift values with appropriate examples.

4.C. Explain the hyperfine ESR spectrum of one electron system coupled with a nuclear spin, I-1.

(4+4+2)

5.A. Identify the Compound B ($C_9H_{10}O_2$) which shows the following mass spectra



The IR main peaks obtained for the same compound appear at 3058, 2941, 1745, 1385, 1225, 1026, 749 and 697 cm^{-1}

The proton NMR data obtained for the same are as follows

Chemical Shift (ppm)	Peak area	Splitting
7.22	5	Singlet
5.00	2	Singlet
1.96	3	Singlet

5.B. Differentiate between two types of continuous wave NMR. Write any two advantages of FTNMR.

5.C. The fragmentation of molecular ion of 2-pentanone gives rise to dominant peaks at m/z=71, 58 and 43

i) Construct a balanced equation to show how fragmentation of the molecular ion give rise to the peak at m/z = 58 using Mc Lafferty rearrangement

ii) Write the structural formula of the fragment with m/z = 43

(4+4+2)

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