BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: MSC **SEMESTER : III**
BRANCH: CHEMISTRY **SESSION : MO/19**

SUBJECT: CH501 SPECTROSCOPIC ELUCIDATION OF MOLECULAR STRUCTURE
TIME: 3 HOURS **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

Q.1(a) Discuss 'solvent effect' in case of UV-VIS spectroscopy of organic molecules. [5]

Q.1(b) Compare and contrast the vibrational spectroscopy of a diatomic molecule when we consider it as 'simple harmonic oscillator' vs the case when considered as 'Anharmonic oscillator'. [5]

Q.2(a) Write a fundamental Equation of NMR to demonstrate the relation between applied magnetic field and radiofrequency. The observed chemical shift of a proton is 912 Hz from TMS and the operating frequency of the spectrometer is 300 MHz. Calculate the chemical shift in terms of δ (ppm). [5]

Q.2(b) An organic compound having molecular formula $C_6H_{11}BrO_2$ exhibits the following peaks in 1H NMR: δ: 4.1 (2H, q, J = 7.5 Hz); 4.0 (2H, t, J = 7.5 Hz), 1.5-2.2 (2H, m,); 1.25 (3H, t, J = 7.5 Hz), Determine the structure. [5]

Q.3(a) Outline with well labelled schematics the Fast Atom Bombardment (FAB) method of generating molecular ions in mass spectroscopy. Discuss the advantages and disadvantages of the FAB technique. [5]

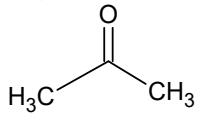
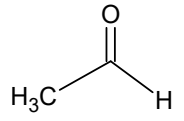
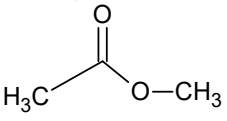
Q.3(b) Outline the competing molecular fragmentation pathways in MS of cyclohexene. Identify the dominant pathway with suitable reason. [5]

Q.4(a) Explain how 'chemical shrift' in Mossbauer spectroscopy of ^{119}Sn is instrumental in determination of oxidation state of 'Sn' in unknown compounds. [5]

Q.4(b) How electric quadrapole effect in Mossbauer spectroscopy can be instrumental in predicting accurate structure of isomers of $I_2Cl_4Br_2$? [5]

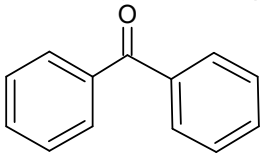
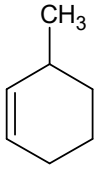
Q.4(C) A free electron is placed in a magnetic field of strength 1.3T. Find out the resonance frequency when g = 2.0023 and Bohr magnetron $\mu_B = 9.274 \times 10^{-24}$ J T^{-1}.

Q.5(a) Arrange in increasing order the 'C=O' stretching frequency for the following compounds. Give reason. [5]

(i)  (ii)  (iii) 

Q.5(b) The base peak of most methyl ketones is at m/z 43. Explain the reason with suitable example. [5]

Q.5(C) Discuss the fragmentation pattern in MS of the following compounds:

(a)  (b) 

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