LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – CHEMISTRY

SECOND SEMESTER – APRIL 2015

CH 821 – MOLECULAR SPECTROSCOPY

Date : 20/04/2015   Dept. No. [   ]   Max. : 100 Marks
Time : 09:00-12:00

Part-A

Answer all questions. Each question carries two marks: *(10x2=20)*

1. Identify the compound C_9H_{12} that shows two singlets in 1:3 ratio in its ^{1}HNMR spectrum.
2. Prove that the operations S_3^1 and S_3^5 belong to the same class.
3. Distinguish between fundamental and hot bands.
4. Identify the point groups of NH_3 and CCl_4 molecules.
5. Mossbauer spectra are recorded as a function of the velocity of the source nucleus. Give reason.
6. State the selection rule for rigid diatomic rotator and pure rotational Raman.
7. Mention the factors which cause bathochromic shift in a molecule.
8. Derive the ground term symbol of nitrogen atom.
9. How will you distinguish between primary and secondary alcohols by NMR technique?
10. How is s/n ratio enhanced?

Part-B

Answer any eight questions. Each question carries five marks:

(8x5=40)

11. Explain diamagnetic anisotropy with an example.
12. Explain the epr spectrum of methyl radical with the hyperfine splitting diagram.
13. Discuss the origin of P, Q, and R branch lines in the vibration-rotation spectra.
14. Explain the use of Woodward-Fieser rules in interpreting the electronic absorption bands of homo- and heteroannular dienes with an example.
15. How will you compare the intensities of Raman vibrational spectral lines of a compound?
16. Outline the construction of character table for C_{3v} point group.
17. Deduce the structure of the compound $C_{10}H_{12}O_2$ from the NMR data: δ 7.26, s, 5H; 4.12 q, 2H; 3.55, s, 2H; 1.22, t, 3H.
18. Explain the effect of isotopic substitution on the rotational spectra of molecules.
19. Deduce the group multiplication table for water molecule.
20. The vibrational wave number for HCl in IR spectrum is 2990cm^{-1}. Calculate zero point energy and the force constant.
21. Discuss Franck-Condon principle to account for intensity variations of spectral transitions.
22. Explain isotopic peaks and metastable peaks with an example.

Part-C

Answer any four questions. Each question carries ten marks: (4x10=40)

23. Explain the mechanism of spin-spin splitting in NMR and isomer shift in Mossbauer spectroscopy.

24a. Discuss the use of infrared spectroscopy to study hydrogen bonding.

(5)

  b. How are IR and Raman spectroscopy helpful in explaining the structure of SO_2 and CO_2 molecules?

(5)

25. Explain McLafferty rearrangement and the influence of solvent on λ_{max} in the UV-Visible spectra of compounds.

26a. Outline the causes for the broadening of spectral lines.

(4)

  b. Describe the effect of the interaction of molecules with photons in the different regions of the electromagnetic radiation.

(6)

27a. Propose the structure for a hydrocarbon which exhibit the molecular ion peak at m/z 102, ^{1}HNMR resonance at 7.4(s,5H) and 3.1(s,1H) ppm, and IR absorptions at 2210 and 3310 cm^{-1}.

(5)

  b. Identify the structure of a liquid (bp 82°C) with mol.wt 60, strong and broad IR absorption at 3300 cm^{-1} and ^{1}HNMRresonance at 1.1(d,6H), 3.9(heptet,1H), and 4.8(s,1H) ppm.

(5)

28a. How many lines are possible in the atomic spectrum of sodium? Mention the energy levels involved in the transitions.

(6)

  b. Calculate the Lande's g-value for the ground state of sodium.

(4)

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