17P315 (Pages: 2) Name: ………….………..

Reg. No…..………….……….

THIRD SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2018
(Regular/Supplementary/Improvement)
(CUCSS - PG)
CC15P CH3 C09 - MOLECULAR SPECTROSCOPY
(Chemistry)
(2015 Admission onwards)

Time : Three Hours   Maximum : 36 Weightage

Part A
Answer *all* questions. Each question carries 1 weightage.

1. Explain the width of a spectral line using Heisenberg Uncertainty principle.

2. How intensity of spectral line is controlled by the population?

3. Explain the method for determining the dipole moment of gaseous molecules.

4. How many normal modes of vibrations are there for benzene molecule?

5. Calculate the value of ν_{max} for HCl when the anharmonicity constant is 0.0174.

6. What is the use of Fortrat diagram in electronic spectroscopy?

7. Explain the reason for applying the external magnetic field in magnetic resonance spectroscopy.

8. Predict the EPR spectrum of pyrazene negative ion.

9. Aniline absorbs at 280 nm in UV-Visible spectra. But its acidic solution shows a bathochromic shift to 208 nm. Explain.

10. A pale yellow organic compound with molecular formula $C_6H_5NO_3$ is found to be showing NMR spectrum with an unsymmetrical multiplet at 1.8 -2.9 τ (4H) and singlet at 0.1τ (1H). Describe the spectrum and predict the structure.

11. How Mossbauer spectroscopy is used to distinguish between $FeSO_4$ and $FeCl_3$?

12. How IR spectroscopy can be used to distinguish between
    a. o- and m- methoxy benzyl alcohol?
    b. phenyl acetate and methyl benzoate?

(12 x 1 = 12 Weightage)

Part B
Answer any *eight* questions. Each carries 2 weightage.

13. In a given organic compound two kinds of protons exhibit signals at 50Hz and at 200Hz using a 60MHz instrument. What will be their relative position using 400 MHz instrument? Also convert the position of signals into delta scale.

14. An organic compound shows only two signals (singlets) in its NMR spectrum. The various signals in mass spectrum are at m/e values 57, 43, 41, and 29. Identify the structure of the compound.

15. Explain the rotation spectrum of symmetric top molecules.

16. Explain McLafferty rearrangement in mass spectra.

17. Explain the various factors affecting the intensity of spectral line.

18. Explain the classical theory of Raman effect.

19. Explain zero field spitting and Kramer Degeneracy in EPR spectroscopy

20. Explain Frank-Condon principle for explaining the intensity of electronic transition.

21. The vibrational spectrum of HCl shows a fundamental at 2886cm^{-1}, the first and the second overtones at 5668cm^{-1} and 8347cm^{-1}. Find the value of equilibrium vibrational frequency and anharmonicity constant.

22. What are the applications of DEPT and INEPT spectra?

23. Explain the origin of chemical shift in NMR spectroscopy.

24. Explain the origin of isomer shift in Mossbauer spectroscopy.

(8 x 2 = 16 Weightage)

Part C

Answer any *two* questions. Each carries 4 weightage.

25. Explain
    a) Principle moments of inertia and classification of molecules based on that.
    b) The polarisability ellipsoid for different vibrational modes of CO_2 and sketch them.

26. Explain quantum mechanically chemical shift and spin-spin coupling to first order approximation for the AX spin system. Using tree diagram method to explain AX_2, AX_3, A_2X_3, AM_2X ($J_{AM} \gg J_{AX}$)

27. How would you understand the electronic spectra of conjugated molecules using particle in a one dimensional box model? Discuss.

28. An organic compound with molecular formula C_4H_9NO gives the following spectral data.

    UV : λ_{max} 220nm

    IR : 3500 (m), 3402 (m), 2960 (w), 1682 (s), 1610 (s).

    ^{1}HNMR: δ 1.0 (doublet), 2.1 (septet), 8.1 (siglet).

    Determine the structure of the compound and explain the spectrum.

(2 x 4 = 8 Weightage)

****