**16P309** (Pages:2) Name……

Reg. No……

**THIRD SEMESTER M.Sc. DEGREE EXAMINATION, OCTOBER 2017**

(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 transition moment integral in spectroscopy. How does it help in predicting the transitions in spectroscopy?
2. Explain Doppler broadening.
3. What is the effect of substituting a hydrogen atom by a deuterium atom in hydrogen molecule on rotational constant B?
4. Define normal mode of vibration
5. Explain Fermi resonance.
6. Explain Predissociation.
7. Explain the reason for applying RF radiation perpendicular to the external magnetic field in magnetic resonance spectroscopy?
8. Predict the EPR spectrum of naphthalene negative ion?
9. M- nitrophenol in neutral solution absorbs at 330nm while in alkaline solution absorbs at 380nm, in contrast p-nitrophenol has absorption maximum at 320nm in neutral solution and 400 nm in alkaline solution. Explain.
10. Predict the number of proton NMR signals in N,N Dimethyl formamide. Explain?
11. Explain ORD with example
12. How IR spectroscopy can be used to distinguish between
    1) o- and m- methoxy benzyl alcohol
    2) 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, 200Hz using a 60MHz instrument. What will be their relative position using 90MHz instrument? Also convert the position of signals into delta scale.
14. Explain how IR spectroscopy can be applied to predict the product formation at each step in the following reaction series.

    Benzaldehyde → Benzoin → Benzil → Benzilic acid.

15. Derive an expression for Jmax for the rigid rotor at which there is maximum population.

16. The fundamental and first overtone transition of $^{14}N^{16}O$ are centred at 1876.06 cm-1 and 3724.20 cm-1 respectively. Calculate the force constant, zero point energy, anharmonicity constant and equilibrium vibration frequency of the molecule.
17. Explain the various factors affecting the width of spectral line.
18. Explain how Octant rule and Axialhaloketone rule is useful for the determination of conformation and configuration of 3-methyl cyclohexanone.
19. Explain zero field spitting and Kramer Degeneracy
20. Explain Frank-Condon principle for explaining the intensity of electronic transition.
21. Explain Nitrogen rule and Rule of Thirteen in mass spectrometry.
22. What are the applications of 2D-COSY spectra?
23. Explain the origin of spin-spin coupling in NMR spectroscopy.
24. Explain with energy level diagram, the magnetic hyperfine interaction in Mossbauer spectroscopy.

**(8 x 2 = 16 Weightage)**

## Part C

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

25. Discuss a) Relaxation methods in NMR spectroscopy and its determination using FTNMR

    b) Nuclear Overhauser Effect and its use in structure elucidation.
26. a) Discuss the use of spin-spin coupling constant values in obtaining stereochemical information in NMR.

    b) Predict the structure of the compound with the following spectral characteristics:

    UV: 290 nm

    IR : 2980, 1718, 1440 cm-1

    1H NMR : 2.3ppm (q), 2.15ppm(s), 1.1ppm(t)

    Mass (m/z) : 72(M+), 43 (base peak), 29
27. How would you understand the electronic spectra of conjugated molecules using particle in a one dimensional box model? Discuss.
28. Define Mossbauer effect. How it is made use of in structural elucidation of co-ordination complexes? Discuss.

**(2 x 4 = 8 Weightage)**

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