19P310 (Pages: 2) Name……..……

Reg. No……..……

THIRD SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2020

(CUCSS - PG)

CC19P CHE3 C09 - MOLECULAR SPECTROSCOPY

(Chemistry)

(2019 Admission - Regular)

Time: Three Hours Maximum: 30 Weightage

Part A

Answer any ***eight*** questions. Each question carries 1 weightage.

1. What are the different classes of molecules based on moment of inertia?
2. State mutual exclusion principle.
3. Explain how microwave spectroscopy can be used for calculating the dipole moment of molecules.
4. What is resonance Raman spectroscopy?
5. Explain Zeeman effect
6. What is meant by transition moment integral?
7. What are the energy levels for a spin I=3/2 system in the presence of an external magnetic field?
8. Predict the EPR spectrum of pyrazine negative ion?
9. What is HMBC and HMQC spectra in NMR spectroscopy?
10. How IR spectroscopy can be used to distinguish between otho hydroxy benzoic acid and meta hydroxy benzoic acid?

(8 x 1 = 8 Weightage)

Part B

Answer any ***six*** questions. Each question carries 2 weightage.

11. How will you determine the bond length of linear triatomic molecule using microwave spectroscopy?
12. A organic compound with molecular formula C3H9N shows the following peaks in the IR spectrum, 1) 3012 cm-1 (m) 2) 3425 cm-1 (s) 3) 3236 cm-1 (m) 4) 1615 cm-1(m). When the compound A is treated with nitrous acid we get a compound B which shows a strong peak at 3430 cm-1. Identify A and B. Also explain the peaks in the IR spectrum.
13. Explain the Karplus equation and how it is used in structural elucidation in NMR spectroscopy.

14. 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.
15. Explain Nuclear Overhauser Effect and its use in structure elucidation.
16. Explain factors responsible for intensity of spectral lines.
17. Briefly explain McLafferty rearrangements.
18. What do you mean by first order and non first order NMR spectra. Explain this using Hamiltonian operators.

(6 x 2 = 12 Weightage)

Part C

Answer any ***two*** questions. Each question carries 5 weightage.

19. Discuss:
    a) Relaxation methods in NMR spectroscopy and its determination using FTNMR
    b) Off-resonance and noise decoupled spectra in NMR
20. a) Discuss the different ionization techniques in mass spectrometry.
    b) Predict the structure of the compound with the following spectral characteristics: Molecular formula: C8H10O; IR peaks at 3010, 2870, 1605, 1510, 1005 and 805cm-1; NMR δ = 2.25 singlet (3H); 3.72 singlet (3H); 6.78 doublet (2H); 7.05 doublet (2H).
21. a) Explain the DEPT and INEPT in NMR.
    b) Explain the Classical and Quantum theory of Raman Effect
22. a) Explain the quantum mechanical description of AX and AB NMR pattern.
    b) Briefly Explain the Zero field splitting and Kramer's theorem in EPR spectroscopy.

(2 x 5 = 10 Weightage)

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