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Name.....

Reg. No.....

# THIRD SEMESTER M.Sc. DEGREE (REGULAR) EXAMINATION NOVEMBER 2019

Chemistry

CH3C09-MOLECULAR SPECTROSCOPY

Time : Three Hours

Maximum: 36 Weightage

# Section A

## Answer all questions.

Each questions carries 1 weightage.

- Discuss the factors influencing bandwidth in vibrational spectrum.
- 2. Vibrational frequency in the excited state of a molecule is smaller than that in the ground state.
  Why?
- 3. Explain Karplus relationship.
- 4. What is Larmor frequency in NMR?
- 5. What is 'g' factor ? How are 'g' values determined ?
- 6. Explain Doppler broadening.
- 7. What is meant by rigid rotor?
- 8. Give examples for spherical top molecules and give the symmetric criteria.
- 9. Why homonuclear diatomic molecule does not give any vibrational spectra ?
- 10. Explain McConnell equation?
- 11. 13C NMR is active while 12C NMR does not. Why?
- Explain high resolution mass spectrometry (HRMS).

 $(12 \times 1 = 12 \text{ weightage})$ 

#### Section B

Answer any eight questions. Each question carries 2 weightage.

- 13. Explain the factors responsible for the hyperfine structure in EPR spectra.
- 14. Give the principle of Optical Rotatory Dispersion and explain Circular Dichroism.
- 15. Write notes on : (i) Predissociation ; and (ii) Fermi resonance.
- 16. What is Nuclear Overhauser Effect (NOE)?

Turn over

- 17. Write a note on cotton effect.
- 18. Detail Franck-Condon principle.
- 19. Determine the principal moment of inertia of methane if its bond length is 1.09 A°?
- 20. Draw a diagram showing the allowed rotational energies of a rigid diatomic molecule and explain?
- Explain the various factors influencing the width and intensity of spectral lines in microwave spectrum.
- 22. Discuss microwave spectroscopy.
- 23. The mass spectrum of 2-butenal shows a peak at m/z 69 that is 28.9 % as intense as the base peak. Propose at least one fragmentation route to account for this peak and explain why this fragment would be reasonably stable?
- 24. Detail the factors affecting the position and intensity of electronic absorption bands?

 $(8 \times 2 = 16 \text{ weightage})$ 

## Section C

# Answer any two questions. Each question carries 4 weightage.

- 25. (a) Write note on FT NMR.
  - (b) Explain the theory of spin-spin splitting in NMR spectroscopy.
- (a) Explain the application of Mossbauer spectroscopic techniques in the study of Fe (II) and Fe
   (III) cyanides.
  - (b) What is isomer shift in Mossbauer Spectroscopy?
- 27. (a) What vibrational frequency in wave number corresponds to a thermal energy of kT at 298K?
  - (b) Why is that in the excited state of a molecule the vibrational frequency is smaller than in the ground state?
- 28. (a) Explain Kramer's theorem in Electron Paramagnetic Resonance?
  - (b) Write a note on McLafferty rearrangement.

 $(2 \times 4 = 8 \text{ weightage})$