



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – CHEMISTRY

THIRD SEMESTER – APRIL 2016

CH 3810 - MOLECULAR SPECTROSCOPY

Date: 28-04-2016
Time: 09:00-12:00

Dept. No.

Max. : 100 Marks

Part-A

Answer ALL questions.

(10 x 2= 20)

1. What is spherical top molecule? Give an example.
2. The frequency of -OH stretching vibration in CH₃OH is 3300 cm⁻¹. Estimate the frequency of -OD stretching vibration in CH₃OD.
3. State Franck-Condon principle.
4. Distinguish between Rayleigh and Raman scattering.
5. Mention the principle of photoelectron spectroscopy.
6. Sketch the ¹H NMR of ethyl alcohol having hydrogen bonding.
7. Predict the spin of ¹⁴N that shows three hyperfine lines in its EPR spectrum.
8. What is pure NQR spectroscopy?
9. Define: Isomer shift.
10. Mention the significance of quadrupole coupling constant.

Part-B

Answer any EIGHT questions.

(8 x 5= 40)

11. Discuss the factors affecting the intensity of the spectral lines.
12. Explain the vibrational energy of a diatomic molecule using Morse curve.
13. The equilibrium vibrational frequency of the iodine molecule is 215 cm⁻¹ and the anharmonicity constant is 0.003. What is the intensity of the hot band $\gamma = 1 \rightarrow \gamma = 2$ relative to that of the fundamental $\gamma = 0 \rightarrow \gamma = 1$, if the temperature is 300 K?
14. Explain the isotopic effect in the rotational spectra.
15. The first rotational line of ¹²C¹⁶O is observed at 3.84235 cm⁻¹ and that of ¹³C¹⁶O is at 3.67337 cm⁻¹. Calculate the atomic weight of ¹³C assuming the mass of ¹⁶O to be 15.9949 and ¹²C as 12.0.
16. Discuss the rotational Raman spectra of a linear molecule with an example.
17. How will you arrive at the structures of H₃PO₃ and H₃PO₂ molecules using ³¹P NMR?
18. Explain the geminal and vicinal coupling with examples.
19. Account for the hyperfine lines shown by high spin Mn(II) complex.
20. Calculate the number of EPR lines possible for d⁸ and d⁷ configurations.
21. How will you account for the quadrupole splitting exhibited by the compound [Fe(CO)₅]?
22. Prove that the quadrupole coupling constant is twice the NQR frequency for a nucleus with spin I = 3/2.

Part-C

Answer any FOUR questions.

(4 x 10= 40)

23. Discuss the Stark effect of a linear and symmetric top molecule using the rotational spectra.
- 24 a. The first three stokes lines in the rotational Raman spectrum of $^{16}\text{O}_2$ are separated by 14.4 cm^{-1} , 25.8 cm^{-1} and 37.4 cm^{-1} from the exciting radiation. Using the rigid rotor model, calculate the value of r_0 . (8)
- b. Distinguish between stokes and antistokes lines. (2)
- 25 a. What are lasers? Explain any two types of lasers with examples. (5)
- b. Explain the significance of finger print region in IR spectroscopy with suitable examples. (5)
26. What is correlation spectroscopy? Discuss the COSY of isobutyl methyl ester.
- 27 a. Explain the importance of the following: i) electric field gradient ii) asymmetry parameter. (6)
- b. Explain the Kramer's degeneracy with an example. (4)
28. State the selection rule for Mossbauer spectroscopy and explain the Mossbauer spectral features of the compounds: i) $[\text{Fe}(\text{CN})_6]^{4-}$ ii) $\text{Sn}(\text{C}_2\text{H}_5)_4$ (5+5)
