LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – **PHYSICS**

THIRD SEMESTER – APRIL 2017

PH 3815- SPECTROSCOPY

Date: 28-04-2017 Dept. No. Max. : 100 Marks
09:00-12:00

Part - A

Answer all the questions: **(10 × 2 = 20)**

1. Give the selection rule for transition from one state to another for a symmetric top molecule.
2. HCl has a B value of 10.593 cm^{-1} and a centrifugal distortion constant of 5.3×10^{-4} cm^{-1}. Estimate the vibrational frequency.
3. How many normal modes of vibration are possible for
   a) HBr b) H_2O c) C_2H_4 d) C_6H_6
4. State the rule of mutual exclusion.
5. What is pre-dissociation?
6. The absorption spectrum of oxygen consists of a series of bands which terminate in continuous absorption at 1761 Å. The zero point energy in the ground state corresponds to 973 cm^{-1} and the difference in potential energy minima for the two electronic states corresponds to 49,800 cm^{-1}. Determine D_e' of O_2 in kcal mol^{-1} (1 cm^{-1}=11.958 J/mol)
7. An NMR signal for a compound is found to be 120 Hz downwards from TMS peak operating at 100 MHz. Calculate its chemical shift in ppm.
8. Define relaxation time in NMR.
9. What is the difference between inelastic scattering and elastic scattering?
10. Write any two applications of SEM.

Part - B

Answer any four of the following questions: **(4 × 7.5 = 30)**

11. a) Discuss the effect of isotopic substitution on the rotation spectrum. (4.5 marks)
    b) The rotational constant of $H^{35}Cl$ is 10.5909 cm^{-1}. What is the value of B for $H^{37}Cl$?
    (H = 1.673×10^{-27} kg, $^{35}Cl = 58.06 \times 10^{-27}$ kg, $^{37}Cl = 61.38 \times 10^{-27}$ kg) (3 marks)
12. On the basis of polarizability, explain the vibrational Raman activity of CO_2.
13. i) What is Fortrat Parabolae? Obtain an expression for band head. (5)
    ii) The band origin of a transition in C_2 is observed at 19,378 cm^{-1} while the rotational fine structure indicates that the rotational constants in excited and ground states are B'=1.7527 cm^{-1} and B''=1.6326 cm^{-1}. Estimate the position of the band head. (2.5)
14. Derive the expression $1 + \upsilon_{max} = \frac{1}{2\chi_e}$; symbols have standard meaning
15. Give the principle of NMR and explain the working of NMR spectrometer.
16. Outline the principle of photoelectron spectroscopy.

Part – C

Answer any four of the following questions: **(4 × 12.5 = 50)**

17. a) What is a non rigid rotator? Obtain the selection rule and the wave number for transition from one state to another for a rigid rotator. (6 marks)

    b) The rotational spectrum of BrF shows a series of equidistant lines 0.71433 cm^{-1} apart. Calculate the rotational constant B and hence the moment of inertia and the bond length of the molecule. Determine the transition which gives rise to the most intense spectral line at room temperature (300 K). Given, Br = 131.03×10^{-27} kg and F = 31.55×10^{-27} kg (6.5 marks)

18. a) Explain Born-Oppenheimer approximation. Describe with theory, the rotation-vibration spectra of diatomic molecule. (9 marks)

    b) The fundamental and first overtone transitions of CO are centered at 2143.3 cm^{-1} and 4260.0 cm^{-1}. Calculate the equilibrium vibration frequency and anharmonicity constant. (3.5 marks)

19. State the principle of ESR. With necessary diagram, explain how it is used to characterize samples.
20. Using family tree method, explain how spectral splitting is taking place in NMR spectroscopy due to coupling of other nuclei. Give examples.
21. Discuss how Doppler Effect and uncertainty principle influence the Mossbauer spectrum. With a block diagram, explain the working of Mossbauer spectrometer.
22. Outline the principle of electron energy loss spectroscopy in detail.

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