

LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034
M. Sc. DEGREE EXAMINATION – PHYSICS
FIRST SEMESTER – NOVEMBER 2003
PH 1804 / PH 725 – SPECTROSCOPY

11.11.2003
1.00 – 4.00

Max. : 100 Marks

PART – A

Answer ALL the questions.

(10 x 2 = 20)

01. How are molecules classified on the basis of moment of inertia? Give one example for each.
02. The moment of inertia of OCS molecule is $137.95 \times 10^{-47} \text{ kg-m}^2$. Calculate the rotation constant.
03. What type of spectroscopy is best suited for H_2 ? Give reasons.
04. Explain with an example, the rule of mutual exclusion.
05. What is Fortrat parabola?
06. The band origin of a transition in C_2 is observed at 19378 cm^{-1} while the rotational fine structure indicates that the rotational constants in excited and ground states are respectively $B^1 = 1.7527 \text{ cm}^{-1}$ and $B^{11} = 1.6326 \text{ cm}^{-1}$. Estimate the position of the band head.
07. Define quadrupole moment of a nucleus.
08. Give the importance of double resonance technique.
09. Calculate the magnetic field strength required to get transition frequency of 60 MHz for hydrogen nuclei.
10. A Mossbauer nucleus has spin $1/2$ and $3/2$ in the ground state and excited state respectively. Sketch the Spectrum when combined electric and magnetic fields are present.

PART – B

Answer any FOUR

(4 x 7.5 = 30)

11. a) Explain the factors that determine the intensity of a spectral line. Obtain an expression for J at which maximum population occurs.

b) The separation between lines in the rotational spectrum of HCl molecules was found to be 20.92 cm^{-1} . Calculate the bond length.
12. a) How many normal modes of vibration are possible for H_2O ? Show by sketch the fundamental vibrational modes of H_2O molecule.

b) Outline the theory of Raman spectrum on the basis of (1) Classical theory and (2) Quantum theory.
13. Explain the importance of Franck-Condon principle in explaining the intensity of molecular Spectrum.
14. Discuss the T_1 and T_2 relaxation mechanism in NMR. Derive an expression for the relaxation time T_1 .
15. Explain with a neat diagram, the functioning of Electron energy loss spectrometer.

PART – C

Answer any FOUR

(4 x 12.5 = 50)

16. (a) Explain, with theory, the spectrum of a linear diatomic molecule of rigid rotor type. Deduce the correction for non-rigid type.
- (b) Calculate the frequency of NO molecule whose force constant is 1609 Nm^{-1} .
17. (a) Explain Born-Oppenheimer approximation. Describe, with theory, the rotation – vibration spectra of a diatomic molecule.
- (b) The fundamental and first overtone transition of ^{14}N , ^{16}O are centered at 1876.06 cm^{-1} and 3724.20 cm^{-1} respectively. Equivalent the equilibrium frequency, anharmonicity constant and zero point energy.
18. Obtain an expression for the Dissociation energy of a molecule. The Vibrational Structure of the absorption Spectrum of O_2 becomes a continuum at $56,876 \text{ cm}^{-1}$. If the upper electronic state dissociates into one ground state atom and one excited atom with excitation energy $15,875 \text{ cm}^{-1}$, estimate the dissociation energy of ground state of O_2 in cm^{-1} and kJ / mole .
19. Explain the principle of ESR. Sketch a neat diagram and explain the functioning of ESR Spectrometer.
20. Outline the importance of 'RAIRS' technique in characterising the absorbed surfaces on a specimen.

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