

PHYSICAL CHEMISTRY - III

(Common with B.Sc. Bio-Technology, Industrial Microbiology)

Time : Three Hours]

[Maximum Marks : 35

Note : Attempt two questions each from Section A and B carrying 7 marks each. Section C is compulsory consisting of 7 short answer type questions carrying 1 mark each.

Section - A

- (a) Discuss the particle in a one-dimensional box. Find expressions for its energy and wave function. 4

(b) Evaluate $\left[x, \frac{d}{dx} \right]$. 3
- (a) Derive an expression for Plank's radiation law. 4

(b) What are Normalized, Orthogonal and Orthonormal wave function ? 3
- (a) Give the postulates of Quantum mechanics. 4

(b) Discuss the spectral distribution of energy in case of black body radiations. 3
- Set up Schrödinger wave equation for Hydrogen and hydrogen-like particles-like particle. Separate into its variables to get three independent equations. 7
- (a) Discuss IR (pure vibrational) spectra for a diatomic molecule by considering it a simple harmonic oscillator. 4

(b) Calculate the force constant K for N₂ molecule. Given that fundamental vibrational frequency is $6.8 \times 10^{13} \text{ s}^{-1}$. 3
- (a) What are normal modes of vibrations of a molecule ? Calculate and draw vibrational degree of freedom for CO₂ and H₂O. 4

(b) The rotational spectral of a diatomic molecule (HCl) shows a series of equidistant lines spaced at 24.6 cm^{-1} . Calculate its band length and moment of inertia.
- (a) What are selection rules in spectroscopy ? Discuss for rotational and vibrational (IR) spectra. 4

(b) Which of the following molecules will show pure rotational and pure vibrational spectra, and why ?

8. (a) HCl, CO₂, NO, Cl₂, HCN, CH₄.
(b) Discuss pure rotational (microwave) spectra of a diatomic molecules. 3
What is Isotopic effect? How does it affect the spacing between the lines in case of rotational spectroscopy? 4

Section - C
(Compulsory Question)

9. Answer in brief:

- (a) Give selection rules for anharmonic oscillation.
(b) How intensity of spectral lines varies in case of a pure rotational spectra?
(c) What is Zero point energy?
(d) "Homomuclear diatomic molecules do not show rotational spectra." Comment.
(e) In which region IR spectrum takes place?
(f) Evaluate $\Psi = \sin x$ for the operation $\frac{d}{dx}$ and find eigen value.
(g) What are Spherical harmonics? (7×1=7)