61903

Reg. No. | | | | | | | | |

I Semester M.Sc. Degree Examination, March/April - 2025

CHEMISTRY

Physical Chemistry - I

(CBCS Scheme 2019-20 Onwards)

Paper : Ch-103

Time : 3 Hours **Maximum Marks : 70**

Instructions to Candidates:

Answer question No. 1 and any Five of the remaining questions.

1. Answer any TEN of the following questions. **(10×2=20)**

a) Given $\hat{A} = 4x^2, \hat{B} = \frac{d}{dx}$ *and* $f(x) = \sin 3x$, verify whether the operators $\hat{A}$ *and* $\hat{B}$ commute with each other.

b) Comment on the eigen functions and eigen values of the angular momentum operator.

c) Calculate the degeneracy of a particle of mass m trapped in a cubical box of dimension 'a' having an energy of $\frac{14h^2}{8ma^2}$.

d) Express the mathematical relation between Cartesian and spherical polar coordinate systems.

e) What is the significance of anti-symmetric electronic wave functions in quantum mechanics?

f) State variation theorem and mention its equation.

g) Differentiate activation energy and threshold energy of a reaction.

h) Predict the effect of ionic strength on the following reations: $S_2O_8^{2-} + I^- \rightarrow$ *products and* $CH_2ICOOH + CNS^- \rightarrow$ Products

[P.T.O.

i) Conventional methods are not adequate to analyze kinetics of fast reactions. Justify.

j) Differentiate energized molecule from activated molecule in the Hinshelwood theory of unimolecular reactions.

k) Write BET equation for estimation of surface area and explain the terms involved in it.

l) What are the salient features of Lineweaver-Burk plot?

2. a) State the postulates of quantum mechanics.

b) Define Hermitian operators. Prove that eigen values of a Hermitian operator are always real. **(5+5)**

3. a) What are radial distribution functions? Plot the radial distribution functions of 3s, 3p and 3d orbitals and mention their salient features.

b) Write a note on JJ coupling. **(6+4)**

4. a) Define activated complex and transition state. Discuss the postulates of transition state theory.

b) Discuss the mechanism and kinetics of photochemical formation of HCl. **(6+4)**

5. a) Explain in detail the limitations of Lindemann theory of unimolecular reactions.

b) Derive Gibbs adsorption isotherm. State its significance. **(5+5)**

6. a) Explain the terms normalization and orthogonality of wave functions.

b) Discuss the application of variation method to particle in a one-dimensional box. **(4+6)**

7. a) Write short notes on i) Laplace equation ii) Kelvin equation.

b) Outline the temperature jump method of analyzing fast reaction kinetics. **(6+4)**

8. a) Apply and solve Schrodinger wave equation to the harmonic oscillator model and obtain an expression for eigen values of energy.

b) Obtain first order correction term to energy using time independent perturbation method. **(6+4)**