LOYOLA COLLEGE (AUTONOMOUS) CHENNAI – 600 034

B.Sc. DEGREE EXAMINATION – **CHEMISTRY**

SIXTH SEMESTER – **APRIL 2025**

UCH 6502 – MOLECULAR DYNAMICS

Date: 26-04-2025   Dept. No.   Max. : 100 Marks
Time: 09:00 AM - 12:00 PM

SECTION A - K1 (CO1)		
	Answer ALL the Questions	**(10 x 1 = 10)**
1.	**Choose the correct answer**	**(5 x 1 = 5)**
a)	The minimum energy required to eject photoelectrons is known as (i) activation energy (ii) kinetic energy (iii) work function (iv) wave function	
b)	The order of the point group, C_{2h} is (i) 4 (ii) 5 (iii) 3 (iv) 6	
c)	The oxidation of luminol by hydrogen peroxide is an example for (i) photosensitisation (ii) chemiluminescence (iii) quenching of fluorescence (iv) bio-luminescence	
d)	The photosensitizer in uranyl oxalate actinometer is (i) UO^{2+} (ii) UO_2^+ (iii) UO_2^{2+} (iv) UO_3^+	
e)	Which adsorption isotherm is applied to study the thermodynamics of adsorption of a solute at the surface of a liquid? (i) Freundlich (ii) Langmuir (iii) BET (iv) Gibbs	
2.	**Answer the following**	**(5 x 1 = 5)**
a)	Find the eigen value of the function, e^{-ax} for the operator d/dx.	
b)	Write the point group of pyridine.	
c)	What is meant by a primary process?	
d)	What are chemical actinometers?	
e)	Name the rule formulated to describe the flocculation of a sol.	
SECTION A - K2 (CO1)		
	Answer ALL the Questions	**(10 x 1 = 10)**
3.	**True or False**	**(5 x 1 = 5)**
a)	The operator corresponding to total energy of a system is called the Laplacian operator.	
b)	The product of any two symmetry operations is also a symmetry operation.	
c)	The photoexcitation in PS II produces a weak oxidant and a strong reductant.	
d)	Flash photolysis is a relaxation technique.	
e)	Freundlich adsorption isotherm is applied only for multilayer adsorption.	
4.	**Define the following**	**(5 x 1 = 5)**
a)	Compton effect	
b)	Class of a group	
c)	Quantum yield	
d)	Static quenching	
e)	Critical micelle concentration	

	SECTION B - K3 (CO2)	
	Answer any TWO of the following	**(2 x 10 = 20)**
5.	(a) State the postulates of quantum mechanics.	
	(b) Find the wavelength in Å of the line in Balmer series that is associated with drop of an electron from the fourth orbit. (R_H = 109600 cm^{-1})	(6+4)
6.	(a) Write the group multiplication table for C_{3v} point group.	
	(b) Derive Stern-Volmer equation.	(5+5)
7.	(a) Illustrate the mechanism of photosensitisation with an example.	
	(b) When irradiated with light of wavelength, 5000 Å, 1×10^{-4} mol of a substance is decomposed. How many photons are absorbed during the reaction if its quantum efficiency is 10.0?	(6+4)
8.	(a) Derive Langmuir adsorption isotherm by stating the assumptions.	
	(b) Write BET equation and mention the terms in it.	(7+3)
	SECTION C – K4 (CO3)	
	Answer any TWO of the following	**(2 x 10 = 20)**
9.	(a) State Wien's and Stefan-Boltzmann laws of blackbody radiation.	
	(b) Explain the optical and mechanical properties of colloids.	(5+5)
10.	(a) Describe the various types of symmetry elements and their corresponding symmetry operations in detail.	
	(b) Identify the symmetry elements and point group of acetylene.	(7+3)
11.	(a) Describe the various factors affecting fluorescence.	
	(b) State (i) Kasha's rule and (ii) Stark-Einstein law.	(6+4)
12.	Explain the kinetics of photochemical formation of HCl from H_2 and Cl_2.	
	SECTION D – K5 (CO4)	
	Answer any ONE of the following	**(1 x 20 = 20)**
13.	(a) Derive time-independent Schrodinger wave equation.	
	(b) State the mathematical rules for the formation of a group.	
	(c) What are isomorphic and abelian groups? Cite examples.	(10+6+4)
14.	(a) Sketch and explain Jablonski diagram to describe the various photophysical processes associated with the absorption of light.	
	(b) Explain ferrioxalate and MGL actinometers.	
	(c) Discuss the applications of colloids.	(10+5+5)
	SECTION E – K6 (CO5)	
	Answer any ONE of the following	**(1 x 20 = 20)**
15.	(a) Obtain the expressions for energy and wave function for a particle in one dimensional box.	
	(b) Calculate the zero point energy of an electron in one dimensional box of length 20 Å.	
	(c) Apply group theory to predict the optical activity and dipole moment of molecules with suitable examples.	(7+5+8)
16.	(a) Write the mechanistic steps in the photophysical kinetics of unimolecular processes.	
	(b) Compare the following with relevant examples.	
	(i) Photochemical and Thermal reactions (ii) Physisorption and Chemisorption	
	(iii) Lyophilic and Lyophobic colloids	(5+15)