LOYOLA COLLEGE (AUTONOMOUS) CHENNAI – 600 034

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

SIXTH SEMESTER – **NOVEMBER 2024**

UCH 6502 – MOLECULAR DYNAMICS

Date: 20-11-2024 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.	**Answer the following**	
a)	State Compton effect.	
b)	Identify the point group of CO_2 molecule.	
c)	What are radiative processes?	
d)	The quantum yield of photochemical formation of HCl is very high compared to HBr formation. Why?	
e)	State Schultz-Hardy rule.	
2.	**Define the following**	
a)	Ultraviolet catastrophe	
b)	Symmetry operation	
c)	Quantum yield	
d)	Quenching	
e)	Lyophobic colloids	
	SECTION A - K2 (CO1)	
	Answer ALL the Questions	**(10 x 1 = 10)**
3.	**True or False**	
a)	Black body radiation curve for different temperature at wavelengths that are directly proportional to temperature.	
b)	The point group of BF3 is C3v.	
c)	A chemical reaction initiated by the absorption of energy in the form of light is often classified as thermal reactions.	
d)	Quenching may also results from the presence of externally added species which takes up energy from the excited state molecule. This is known external quenching.	
e)	Brownian motion refers to the proper movement displayed by small particles that are suspended in fluids.	
4.	**Match the following**	
a)	Malachite green - $C_{\infty v}$	
b)	Delayed fluorescence - Photoelectric effect	
c)	HCl molecule - Adsorbate	
d)	Threshold frequency - Actinometer	
e)	Water molecule - Phosphorescence	
	SECTION B - K3 (CO2)	
Answer any TWO of the following		**(2 x 10 = 20)**
5.	(a) When light of wavelength 3500 Å falls on a metal surface, photo electrons are emitted from it. Find the threshold wavelength and kinetic energy of the emitted electrons. (Given: the work function for metal is 4.65 eV). (4)	
	(b) Illustrate Planck's quantum theory of radiation. (6)	

6.	(a) What is the wave length of light absorbed when an electron in a linear molecule of 10 Å long makes a transition from the energy level n = 1 to n = 2? (3) (b) Show that C_{2v} point group is an abelian group. (4) (c) Calculate the ground state energies of the electron in eV in case of H^+ and Be^{3+} species assuming that their Rydberg constants are equal (R_H = 13.60 eV). (3)

7.	(a) A sample of gaseous HI was irradiated by light of wavelength 2537 Å where 307 J of energy was found to decompose 1.30 x 10-3 mol of HI. Calculate the quantum yield for the dissociation of HI. (4) (b) Illustrate the following: (i) Chemiluminescence (ii) Bioluminescence (3+3)
8.	Illustrate the following: (i) BET equation (ii) Zeta potential (iii) Tyndall effect. (3+4+3)
	SECTION C – K4 (CO3)
Answer any TWO of the following	**(2 x 10 = 20)**
9.	(a) State the postulates of quantum mechanics. (7) (b) Show that √ is not a linear operator. (3)
10.	(a) What is group? Explain the conditions for forming a group and isomorphic group with suitable examples. (6) (b) Explain the failures of classical mechanics. (4)
11.	Explain the photophysical pathway of an electronically excited molecule using Jablonski diagram.
12.	(a) Point out the principle involved in flash photolysis technique. (5) (b) Explain the phenomenon of reverse micelles and critical micelle concentration. (5)
	SECTION D – K5 (CO4)
Answer any ONE of the following	**(1 x 20 = 20)**
13.	(a) Deduce the expression of wave function and energy for a particle in a one-dimensional box of length L. (8) (b) What are classes? Identify the order and number of classes present in the water molecule. (7) (c) Show that the function $\exp(5x^2)$ is an eigen function of the operator, $\frac{d^2}{dx^2}$ and find the eigen value. (5)
14.	(a) State the laws of photochemistry. (6) (b) Discuss the kinetics of photochemical H_2-Br_2 reaction. (7) (c) Derive Stern-Volmer equation. Give its applications. (7)
	SECTION E – K6 (CO5)
Answer any ONE of the following	**(1 x 20 = 20)**
15.	(a) Derive time-independent Schrodinger wave equation. (8) (b) What is group multiplication table? Write the group multiplication table for C2v point group. (7) (c) Illustrate the importance of point group in predicting dipole moment and optical activity of the molecules. (5)

16.	Write the following in detail: (i) Langmuir and Freundlich adsorption isotherms (7+5+8) (ii) Chemical actinometers (iii) Applications of colloids	
