PG/IIS/CEM/201/25

M.Sc. 2nd Semester Examination, 2025

CHEMISTRY

PAPER – CEM-201

Full Marks : 50

Time : 2 hours

Answer **all** questions

The figures in the right hand margin indicate marks

Candidates are required to give their answers in their own words as far as practicable

GROUP–A

Answer any **four** of the following questions : 2×4

1. Define autocatalytic reaction with an example.

2. The following reaction occurs in aqueous solution

$$CH_2ClCOO^- + OH^- \rightarrow CH_2OHCOO^- + Cl^-$$

deduce qualitatively

(*i*) The effect on the rate of increasing dielectric constant (ε)

(*ii*) The sign of entropy of activation.

3. Use energy balance equation to explain the appearance of Stockes and anti-Stokes Raman scattering.

4. Rotational Raman shift is twice as that of rotation frequecy of the molecule. Explain.

5. Position of minimum of potential curve of a SHO is at $x = 0$. Find the position of maximum of its ground state wave function. How does it differ from a classical Harmonic oscillator ?

6. The trial wave functions, $\phi_1 = c_1 x(1-x)$ and $\phi_2 = c_1 x(1-x) + c_2 x^2 (1-x)^2$ give the ground state energies E_1 and E_2 respectively for a particle moving in a 1-D box. If the exact energy is E_0, then arrange E_1, E_2 and E_0 according to their increasing order with justification.

GROUP–B

Answer any **four** questions of the following : 4×4

7. Deduce the following expression for a linear Harmonic Oscillator,

$$a^\dagger |n> = \sqrt{n+1}\,|n+1>$$

and hence show that,

$$\left|n> = \frac{(a^\dagger)^n}{\sqrt{n!}}\right| 0>$$

(symbols have their usual significances).

8. Show that in the *n*th eigen state of a Harmonic Oscillator, the average kinetic energy (<T>) is equal to the average potential energy (<V>). Comment on your result.

9. What is meant by MASER ? Use Einstein's treatment of absorption and emission phenomena to explain that even ambient or higher temperature is favourable to observe MASER.

10. Give the classical explanation of Raman scattering. State it's drawback. How was it resolved using the concept of quantum mechanics ?

11. Derive the expression for relaxation time of the reaction

$$A + B \rightleftharpoons X$$

Where A and B have different initial concentrations.

12. Antibiotic resistant bacteria have an enzyme, penicillinase, that catalyzes the decomposition of the antibiotic. The molecular mass of penicillinase is 30,000 g mol^{-1}. the turnover number of the enzyme at 28°C is 2000 s^{-1}. If 6.4 μg of penicillinase catalyzes the destruction of 3.11 mg of amoxicillin, an antibiotic (molecular mass 364 g mol^{-1}), in 20 seconds at 28°C, how many active sites does the enzyme have ?

GROUP–C

Answer any **two** questions of the following : 8×2

13. What do you mean by enzyme inhibition ? Discuss different types of enzyme inhibition processes in details. $2 + 6$

14. (*a*) State Franck-Condon principle. Use this principle to explain the relative intensities

of vibronic transition of a diatomic molecule when

(*i*) $r''_e = r'_e$, (*ii*) $r'_e >> r'_e$.

r''_e and r'_e are the position of minima of the ground and excited state potential energy curve respectively.

(*b*) Show that Stokes and Anti-stokes rotational Raman lines are Equi-spaced with respect to the central Rayleigh Scattered line. 1 + 3 + 4

15. (*a*) State and proof Eckart's theorem.

(*b*) Use $\varphi = Ae^{-ax^2}$ as trial wavefunction for the ground state of a linear harmonic oscillator and hence deduce the normalized wavefunction and energy for its ground state. ('A' is the normalization constant and 'α' is the variational parameter) 3 + 5

16. Use linear Harmonic Oscillator model to deduce the essential criteria and the selection rule for a diatomic molecule undergoing transition from the vibrational quantum level v to v'. Recursion relation of Hermite polynomials is given below, 8

$$\xi H_v(\xi) = v H_{v-1}(\xi) + (1/2) H_{v+1}(\xi)$$

[Internal Assessment — 10 Marks]