

SAVITRIBAI PHULE PUNE UNIVERSITY
Progressive Education Society's
Modern College of Arts, Science and Commerce, Ganeshkhind, Pune-411016
B.Sc. Blended Program
(A degree of Savitribai Phule Pune University equivalent to the degree of University of Melbourne)

End Semester Examination: October/November 2024

Program: B.Sc. Blended **Program (Specific):** B.Sc. Blended(Chemistry) **Set: A**

Class: T.Y. B.Sc. Blended

Semester: V

Course code: CHM501

Course name: Chemical kinetics, Thermodynamics & Quantum Chemistry

Credits: 3

Time: 2½ hours

Maximum marks: 50

Instructions to the candidate:

- All questions are compulsory.
- Figures to the right indicate marks.
- Draw diagrams wherever necessary.
- Use of scientific calculator is allowed.
- Ask for graph paper if needed.

Q.1] Choose the correct option (Solve ANY 10 out of 12)

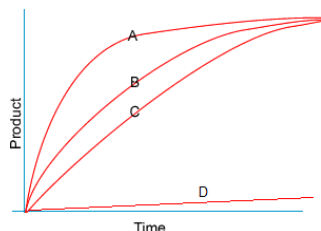
[1 x 10 =10M]

1. The order of the reaction having rate law $\text{Rate} = k[A]^0 [B]^{1/2}$ is —

- a. 3
- b. 5/2
- c. 1/2
- d. 5

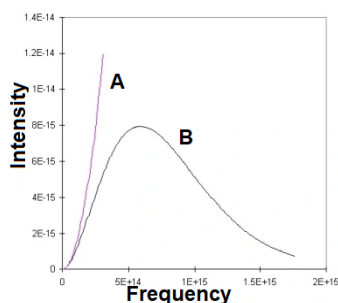
2. The decrease in concentration with respect to time is shown in the diagram.

Identify curve representing the slowest reaction among A, B, C and D.



- a. Curve C
- b. Curve A
- c. Curve D
- d. Curve B

3. In equation $\lambda = h/mv$, the λ represents ----- .
- Only momentum
 - Both particle and wave
 - De Broglie wavelength
 - Only velocity
4. In the equation $\hat{H}\Psi = E\Psi$, H is known as the ---.
- Eigen value
 - Entropy
 - Eigen function
 - Enthalpy
5. The photochemical reaction $\text{H}_2 + \text{Cl}_2 \xrightarrow{h\nu} 2\text{HCl}$ follows --- order kinetics.
- first
 - second
 - third
 - zero
6. In the following diagram, UV catastrophe is represented by -----.



- Graph A
- Graph B
- both A and B
- None of these

7. The ratio of number of photons emitted with the total number of photons absorbed is known as ---
- Quantum number
 - Quantum yield
 - Percent yield
 - Photon ratio
8. Among the following, ---- is the Cp calculated from the rotational partition function.
- R
 - 2R
 - $3/2 R$
 - $5/2 R$

9. The equation $\log N! = N \ln N - N$ represents ----.
 - a. Steady state approximation
 - b. Number approximation
 - c. Stirling approximation
 - d. Molar correction
10. Majority of the quenching in a photochemical reaction is due to the ---.
 - a. Ionisation reaction
 - b. Excitation of the radicals
 - c. Stabilisation of the radicals
 - d. Charge transfer
11. The equation $\int \Psi^* \Psi d\tau = 0$ shows the condition for ----- of the wavefunctions.
 - a. orthogonality
 - b. normalisation
 - c. eigen values
 - d. tunneling
12. The dimensions of the rate constant of the second order reaction ---
 - a. time^{-1}
 - b. $\text{Concentration}^{-1} \text{time}^{-1}$
 - c. $\text{Concentration}^{-2} \text{time}^{-1}$
 - d. $\text{Concentration} \text{time}^{-1}$

Q.2] Answer the following in short (ANY 10 out of 12)

[2 x 10 = 20M]

1. Calculate the degree of freedom for the one component system having equilibrium with three phases.
2. Calculate the de Broglie wavelength of a particle moving with a velocity of $1.3 \times 10^7 \text{ m/s}$ having mass $2.7 \times 10^{-31} \text{ kg}$. Given: Plank's constant (h) = $6.6 \times 10^{-34} \text{ J.s}$
3. Calculate the rate constant of the first order reaction where the initial rate and concentration of the reaction are $4.7 \times 10^{-3} \text{ mol L}^{-1} \text{s}^{-1}$ and 0.025 M respectively.
4. Explain the equation $E = h\nu$.
5. Differentiate between canonical and grand canonical ensembles.
6. Calculate the rotational partition function for a symmetric molecule where $\frac{8\pi^2 I K T}{h^2}$ is 2.108 units.
7. Calculate the degeneracy for the particle in 3-D box with $n^2 = 17$.
8. Explain any one failure of classical mechanics.
9. Discuss the effect of temperature on the photochemical process.
10. Draw a schematic phase diagram of water.

$$\frac{8\pi^2 I K T}{h^2}$$

11. For the reaction ; $2A + B \rightarrow A_2B$,
 Rate = $k [A][B]^2$ with $k = 4.67 \times 10^{-6} \text{ M}^{-2} \text{ s}^{-1}$ at 300K
 Calculate the rate of the reaction when $[A] = 0.5 \text{ M}$; $[B] = 0.2 \text{ M}$.
12. Explain the mathematical expression for partition function.

Q.3. Answer in brief (ANY 4 out of 6)

[4 x 5 = 20M]

1. The data collected for the reaction $2\text{N}_2\text{O}_5 \rightarrow 4\text{NO}_2 + \text{O}_2$ is given below.

Time (s)	0	400	800	1200	1600	2000	2400	2800	3200
$[\text{N}_2\text{O}_5]$	1.63	1.36	1.14	0.92	0.78	0.65	0.52	0.43	0.35

Show that the reaction follows first order kinetics from the graph of $\ln[\text{N}_2\text{O}_5]$ vs Time,

2. Calculate the rate constant and half life of the first order reaction at 500K where its activation energy is 100000 J/mol and pre exponential factor A is $10 \text{ M}^{-1}\text{s}^{-1}$.
3. Calculate the number of microstates for the 14 particles having following distribution

Energy	E_1	E_2	E_3	E_4
Number of particles	2	4	3	5

4. Explain the laws of photochemistry.
5. Derive time independent Shrödinger equation for free particle and explain the terms in it.
6. Derive an expression for the translational partition function, for E, H and Cp and Cv.

-X-