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**F - 307**

**M.Sc. (First Semester)**  
**EXAMINATION, Dec. - Jan., 2021-22**  
**CHEMISTRY**  
**Paper Third**  
**(Quantum Chemistry, Thermodynamics and**  
**Chemical Dynamics-I)**

*Time : Three Hours]**[Maximum Marks:80**[Minimum Pass marks :16*

Note : Attempt all sections as directed

**Section - A**  
**(Objective/Multiple Choice Questions)**  
**(1 mark each)**

Note: Attempt all questions as directed.

Choose the correct answer.

1. Consider the vectors  $u = i - 7j + 3k$  and  $v = -3i + 4j + 2k$ ,  
 sum of these two vectors is:
- (A)  $-4i - 11j + 5k$
- (B)  $2i + 3j + k$
- (C)  $-2i - 3j + 5k$
- (D)  $4i - 3j + 5k$

2.  $\int \left( x^2 + \frac{2}{x^3} - 7 \right) dx = ?$

(A)  $\frac{x^3}{3} + \frac{2}{x^2} - 7$

(B)  $\frac{x^3}{3} - \frac{2}{x^2} - 7$

(C)  $\frac{x^3}{3} - \frac{1}{x^2} - 7x$

(D)  $\frac{x^3}{3} - \frac{1}{x^2} - 7x + c$

3. Which of the following is not a vector quantity?

- (A) Potential energy
- (B) Weight
- (C) Nuclear spin
- (D) Momentum

4. If there exist more than one eigen function corresponding to a given eigen value, then the eigen value is called.

- (A) Nondegenerate
- (B) Degenerate
- (C) Discrete
- (D) Continuum

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5. The zero - point energy for simple harmonic oscillator is  
 $E = \dots\dots\dots$  (where  $h$ - Plank's constant and  $\omega$  - oscillation frequency)
- (A)  $\hbar\omega$   
 (B)  $1/2 \hbar\omega$   
 (C)  $3/2 \hbar\omega$   
 (D)  $5/2 \hbar\omega$
6. Gibbs - Duhem equation relates composition with \_\_\_\_\_ at constant temperature & pressure in liquid phase -
- (A) Fugacity  
 (B) Partial pressure  
 (C) Activity coefficient  
 (D) (A), (B) and (C)
7. The ratio of chemical potential to free energy of a pure substance at constant temperature and pressure is:
- (A) Zero  
 (B) 1  
 (C)  $\infty$   
 (D) None of these
8. Which of the following Maxwell relation is not correct:
- (A)  $dU = TdS - PdV$   
 (B)  $dH = TdS + VdP$   
 (C)  $dF = SdT + PdV$   
 (D)  $dG = VdP - SdT$

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9. Partial molar free energy of an element A in solution is same as its:
- (A) Fugacity  
 (B) Activity  
 (C) Activity coefficient  
 (D) Chemical potential
10. Partial molar quantities are important in the study of:
- (A) Ideal gases  
 (B) Non - ideal mixtures  
 (C) Ideal Solutions  
 (D) A pure component
11. The ionic strength of  $K_2SO_4$  is:
- (A) 1  
 (B) 2  
 (C) 3  
 (D) 4
12. Which one of the following is a second - order reaction?
- (A)  $CH_3COOCH_3 + N_aOH \rightarrow CH_3COON_a + H_2O$   
 (B)  $H_2 + Cl_2 \rightarrow 2HCl$   
 (C)  $2NH_3(g) \rightarrow N_2(g) + 3H_2(g)$   
 (D)  $H_2 + Br_2 \rightarrow 2HBr$
13. For an ideal gas, the activity coefficient is:
- (A) Directly proportional to pressure  
 (B) Inversely proportional to pressure  
 (C) Unity at all pressures  
 (D) None of these

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14. According to Debye - Huckel theory of strong electrolytes, and ion moving in an atmosphere of oppositely charged ions experiences a drag, this effect is known as:
- Asymmetric effect
  - Electrophoresis effect
  - Inter - Ionic effect
  - Concentration effect
15. How many times will the rate of the elementary reaction  $3X + Y \longrightarrow X_2Y$  Change if the concentration of the substance X is doubled and that of Y is half:
- $r_2 = 4.5r_1$
  - $r_2 = 5r_1$
  - $r_2 = 2r_1$
  - $r_2 = 4r_1$
16. The rate constant of the reaction is  $k = 3.28 \times 10^{-4} s^{-1}$ , Find the order of the reaction is:
- Zero order
  - First order
  - Second order
  - Third order
17. In chemical reaction, the rate of reaction increases with temperature, because:
- The kinetic energy of reactants increases
  - The number of collisions between molecules increases
  - Of increases in the number of molecules with the activation energy
  - Of decreases with the activation energy

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18. In Arrhenius plot, intercept is equal to:
- $\ln A$
  - $\log_{10} a$
  - $\ln K$
  - None of these
19. The unit of rate constant for the reaction  $2H_2 + 2NO \rightarrow 2H_2O + N_2$  Which has rate =  $K [H_2][NO]^2$ , is:
- $s^{-1}$
  - $mol^{-2} L^2 s^{-1}$
  - $mol L^{-1}$
  - $mol L^{-1} s^{-1}$
20. In terms of the collision theory of chemical kinetics the rate of a chemical reaction is proportional to:
- The number of collisions per second
  - The number of product molecules
  - The change in temperature per second
  - The change in energy per second

**Section - B****(Very Short Answer Type Question)****(2 marks each)**

Note: Attempt all questions

- If  $e^{x-y} = xy$ , then  $\frac{dy}{dx}$  is.
- Describe two postulates of quantum mechanics.
- Explain the term of fugacity. How it is related to pressure and temperature.?

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- Describe Vant's Hoff reaction isotherm?
- Calculate the ionic strength of a solution that is 0.10 M in  $\text{FeCl}_2$  and 0.20 M in  $\text{FeCl}_3$ .
- Give one method of determination of activity coefficient.
- Explain activated complex theory of reaction rate.
- What is steric factor?

### Section - C

#### (Short Answer Type Questions)

(3 marks each)

**Note: Attempt all questions.**

- Solve the following by differentiation:

$$y = \frac{1}{\sqrt{1-x^2}}, \text{ then } dy/dx = ?$$

- Evaluate  $\int 2 \times (1-x^2)^5 dx$
- An electron is bound in one dimensional box of size  $4 \times 10^{-10}$  m. What will be its minimum energy? (Given:  $m = 9.1 \times 10^{-31}$  kg).
- Derive the Maxwell relation for the following fundamental equation  $(\partial T / \partial V)_S = -(\partial P / \partial S)_V$
- Derive the value of chemical potential of a mixture of ideal gases.
- Find the sum of the three vectors A (1,1,2), B (-1,2,-3), and C (2,-1, 0) with the magnitude and angles of resultant vector of summation.
- Explain Debye - Huckel limiting law.
- What is steady state kinetics? Explain

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### Section - D

#### (Long Answer Type Questions)

(5 marks each)

- Derive, the equation of time independent Schrodinger equation for particle in one dimensional box.

OR

Explain the application of Schrodinger equation for simple harmonic oscillator.

- Define the term of activity. Describe any method for the determination of activity? How Chemical potential vary with pressure.

OR

Explain partial molar properties and partial molar heat content of system. Derive Gibbs- Duhem equation.

- What do you understand by thermodynamics of electrified interfaces? Explain Lippmann equation for surface excess.

OR

Derive the Debye-Huckel- Onsager equation and validity of Onsager's equation for aqueous solution.

- Discuss the kinetics of chain reaction between  $\text{H}_2$  and  $\text{Br}_2$  and derive the rate law.

OR

What are the kinetic and thermodynamic requirements for Chemical oscillation? Explain briefly Belousov - Zhabotinsky (B-Z) Reaction.