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ROLL NO.....

CHE. 203/21

II SEMESTER EXAMINATION, 2021

M.Sc. (CHEMISTRY)

PAPER-III

**QUANTUM CHEMISTRY, THERMODYNAMICS AND
CHEMICAL DYNAMICS - II**

TIME: 3 HOURS

MAX.- 80

MIN.- 16

Note: The question paper consists of three sections A, B & C. All questions are compulsory.
Section A- Attempt all multiple choice/answer in one word questions.
Section B- Attempt one question from each unit.
Section C- Attempt one question from each unit.

SECTION 'A'

2 × 8 = 16

Multiple Choice Questions/ Answer in one word

1. It \hat{A} & \hat{B} are two operators such that $[\hat{A} \hat{B}] = 1$, then what is the result at $[\hat{A}^2 B]$ & $[\hat{A} \hat{B}^2]$ -
(a) $2\hat{B}, 2\hat{A}$ (b) $4\hat{B}, 4\hat{A}$
(c) $4\hat{A}, 4\hat{B}$ (d) $2\hat{A}, 2\hat{B}$
2. Find the inverse of matrix of $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$
(a) -1 (b) -2
(c) -3 (d) -4

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3. Thermodynamic equilibrium involves –
- (a) Chemical equilibrium (b) Thermal equilibrium
(c) Mechanical equilibrium (d) All the above
4. The reaction $\frac{1}{2} N_2(g) + \frac{3}{2} H_2(g) \rightarrow NH_3(g)$ will be attended by -
- (a) Decrease of entropy
(b) Increase of entropy
(c) No change in entropy
(d) Always the entropy remain same
5. Which is not true for a standard hydrogen electrode?
- (a) The hydrogen ion concentration is 1M.
(b) Temperature is 25°C
(c) Pressure at hydrogen is 1atm.
(d) It contains a metallic conductor which does not absorb hydrogen.
6. The potential difference between fixed charged layer and the diffused layer having opposite charge is called-
- (a) Zeta potential (b) Colloidal potential
(c) Dorn potential (d) Streaming potential

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UNIT-II

- Q. 2. Discuss how fugacity vary with temperature & pressure.

OR

Explain the phenomenological law & Onsager's reciprocity relation.

UNIT-III

- Q. 3. Derive the Butler-Volmer equation.

OR

Explain the effect of light at semiconductor solution interfaces.

UNIT-IV

- Q. 4. Describe the theory of Lindemann-Hinshelwood for unimolecular reaction.

OR

Write notes on relaxation methods.

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7. Which of the following statement is true-
- (a) RRKM theory is a canonical transition state theory.
 - (b) RRKM theory is the correction between statistical biomolecular rate theory and the transition.
 - (c) RRKM theory is a microcanonical transition state theory.
 - (d) RRKM consider the following mechanism for a reaction to occur $A^* \rightarrow$ products.
8. Which of the following are true for Hinshelwood –Lindeman theory-
- (a) K_1 increase with S and K_2 decrease with S
 - (b) K_1 and K_2 both decrease with S
 - (c) K_1 and K_2 both increase with S
 - (d) K_1 decreases with S and K_2 increases with S

SECTION 'B' $4 \times 6 = 24$

Short Answer Type Questions (Word limit 200-250 words.)

UNIT-I

Q. 1. $A = \begin{bmatrix} 2 & 1 & 0 \\ 2 & 3 & 1 \\ 1 & 1 & 1 \end{bmatrix}$ & $B = \begin{bmatrix} 1 & 1 & 0 \\ 3 & -1 & 2 \\ 2 & 1 & 3 \end{bmatrix}$

Find out (i) A-B (ii) AB

OR

What are determinants? Define.

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UNIT-II

Q. 2. What is meant by activity?

OR

Write short notes on phenomenological law.

UNIT-III

Q. 3. Explain Gouy-Chapman interface.

OR

Write short notes on hydrogen electrode.

UNIT-IV

Q. 4. What is the flash photolysis?

OR

What is meant by probing the transition state?

SECTION 'C' $4 \times 10 = 40$

Long Answer questions (Word limit 400-450 words.)

UNIT-I

Q. 1. Discuss the linear variation principle.

OR

Explain the first order perturbation theory.