CHE. 203/22

II SEMESTER EXAMINATION, 2022

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' $2 \times 8 = 16$

Multiple Choice Questions/ Answer in one word

1. It $A = \begin{bmatrix} 2 & 4 & -1 \\ -1 & 0 & 2 \end{bmatrix}, B = \begin{bmatrix} 3 & 4 \\ -1 & 2 \\ 2 & 1 \end{bmatrix}$ the find $(AB)^T$, where

    T=transpose of matrix -

    (a) $\begin{bmatrix} 0 & 1 \\ 15 & -2 \end{bmatrix}$ (b) $\begin{bmatrix} 15 & 2 \\ 13 & 1 \end{bmatrix}$

    (c) $\frac{1}{6}\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ (d) None of thse

2. Evaluate $\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$

    (a) 0   (b) 1   (c) 2   (d) 3

3. What is the entropy of the system at equilibrium state?
   (a) zero
   (b) minimum
   (c) maximum
   (d) constant but not maximum

4. In general the transport phenomenon for one dimensional system is written as -
   (a) $J = LX$
   (b) $L = JX$
   (c) $X = JL$
   (d) $J = L/X$
   where J=flux; X=driving force or gradient and L= transport coefficient

5. 'Tafel plot' is the graph between -
   (a) Logarithm of the current density Vs EMF
   (b) Logarithm of the current density Vs. Over potential
   (c) Logarithm of the over potential Vs resistance
   (d) Voltage Vs density

6. In 'Butler-Volmer equation' the graph is plotted between –
   (a) Over potential Vs. resistance
   (b) Current density Vs over potential
   (c) Current density Vs EMF
   (d) Voltage Vs density

UNIT-II

Q. 2. What is fugacity? Discuss the methods used to determine its values. Explain clearly that the fugacity of a gas can be less than as well as more than the pressure.

OR

What is meant by entropy production? Explain the entropy production with specific examples.

UNIT-III

Q. 3. Define 'Overpotential'. Discuss the theories of Overpotential. Explain the various factors affecting it.

OR

Discuss various theories of structure of electrical double layer interfaces in detail.

UNIT-IV

Q. 4. What are fast reaction? Discuss 'Nuclear magnetic resonance and flow method' for the study of fast reaction.

OR

Derive an expression to calculate the value of 'K' with the help of modification made by Marcus in the RRK theory.

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7. An example of a 'Relaxation method of measuring fast reaction rates is' -
   - (a) Spectroscopic monitoring of products
   - (b) Stopped flow technique
   - (c) Temperature Jump experiments
   - (d) Flash photolysis

8. 'Flash photolysis' method for measuring fast reaction rate was developed by-
   - (a) Pinnavaia and Lott
   - (b) Eigen and co-workers
   - (c) Norrish and Porter
   - (d) Roughton and Hastridge

SECTION 'B' $\boxed{4 \times 6 = 24}$

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

UNIT-I

Q. 1. Explain Eigen values of angular momentum.

OR

Write a short note on Ladder Operator for angular momentum.

UNIT-II

Q. 2. Explain the fundamental concept of 'Force and Fluxes' in brief.

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OR

Discuss entropy production in 'Coupled reaction' in brief.

UNIT-III

Q. 3. Explain 'Exchange current density' in brief.

OR

Explain 'Stern model' for electrified interface in short.

UNIT-IV

Q. 4. Discuss the dynamics of barrier less chemical reaction in solutions, in brief.

OR

Explain the dynamics of molecular motion with an example.

SECTION 'C' $\boxed{4 \times 10 = 40}$

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

UNIT-I

Q. 1. What is variation theorem? Discuss the application of variation theorem to Helium atom.

OR

What is angular momentum? Describe it in details.