ED-307

M.Sc. 1st Semester
Examination, March-April 2021

CHEMISTRY

Paper - III

Quantum Chemistry : Thermodynamics and Chemical Dynamics - I

Time : Three Hours] [*Maximum Marks* : 80

Note : Answer **all** questions. The figures in the right-hand margin indicate marks.

Unit-I

1. (*a*) Find the inverse of the matrix 5

$$A = \begin{bmatrix} 3 & -2 & -1 \\ -4 & 1 & -1 \\ 2 & 0 & 1 \end{bmatrix}$$

(*b*) Outline the variation method used for obtaining approximate value of ground state energy system. 5

(*c*) What are the various methods for obtaining approximate solution to the wave function equation ? Discuss the perturbation method and application of first order perturbation theory of the atom. 10

OR

(*a*) Find the inverse of the matrix 5

$$\begin{bmatrix} 5 & -2 & 3 \\ 4 & -1 & -5 \\ 6 & 7 & 9 \end{bmatrix}$$

(*b*) Explain angular momentum operator. Work out measurable value of the angular momentum of the particle. 5

(*c*) Describe eigen value and matrix element of angular momentum operator. 10

Unit-II

2. (*a*) What is partition function ? Discuss rotational partition function. 5

(*b*) Describe Maxwell's thermodynamical relation and discuss its application in proving $C_p - C_v = R$. 15

OR

(*a*) Explain partial molar volume and partial molar heat content. 5

(*b*) What is the most probable distribution ? Explain Maxwell-Boltzmann distribution law of energy partition. Compare it with Bose-Einstein statics. 15

Unit-III

3. (*a*) Write notes on the following : 10

(*i*) Activity coefficient

(*ii*) Electro-catalysis

(*b*) Explain electrical double layer. Discuss Gouy-Chapman electrical double layer. 10

OR

(*a*) Describe the following : 10

(*i*) Ionic strength

(*ii*) Over potential

(*b*) Discuss Debye-Huckel theory for acticity coefficient of electrolytic solution. 10

Unit-IV

4. (*a*) What are the fast reactions ? Describe flash photolysis method of studying fast reaction. 10

(*b*) Discuss the following : 10

(*i*) Activated complex theory

(*ii*) Oscillatory reactions

OR

(*a*) Describe Lindemann's theory of unimolecular reactions. 10

(*b*) Discuss the following : 10

(*i*) Secondary salt effect

(*ii*) Rate expression for the photochemical reaction of H_2 and Br_2