FD-307

M.Sc. 1st Semester
Examination, Dec.-Jan., 2021-22

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*) Transform the complex number, $z = -3 + 2i$ into polar form.   5

   (*b*) If $\vec{r}$ is the radius vector and $\vec{p}$ is the momentum vector and $\vec{L} = i\vec{L}_x + j\vec{L}_y + k\vec{L}_z$ where, $\vec{L}$ is the total angular momentum, then find the values of $\vec{L}_x$, $\vec{L}_y$ and $\vec{L}_z$.   5

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(2)

(c) Give the application of Schrodinger wave equation to find out energy and spherical harmonics of a rigid rotator.   10

OR

(a) If $z_1 = 2 - 3i$ and $z_2 = -5 + 2i$, then find the values of $|z_1|$, $|z_2|$ and the arguments of z_1 and z_2.   5

(b) Write the postulates of quantum mechanics. Derive time independent equation on the basis of postulates of quantum mechanics.   10

(c) Find

$$\int e^{3x} \cos(3x)\, dx$$ 5

Unit-II

2. (a) Using Maxwell relations, show that for van der Waal's gas $\dfrac{\delta Cp}{\delta p} = \dfrac{2a}{RT^2}$.   10

(b) Derive Gibb's-Duhem equation.   5

(c) What is Fugacity ? How it vary with pressure ?   5

OR

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(3)

(a) Show that chemical potential of a component in the gaseous mixture is always less than its chemical potential in the pure state.   10

(b) Give the method of determination of partial molar volume.   5

(c) What is activity ? Discuss activity of an ideal gas and that of a real gas.   5

Unit-III

3. (a) Discuss briefly Debye-Huckel theory of strong electrolytes and give Debye-Huckel Onsager equation.   10

(b) How the mean activity coefficients of electrolytes can be determined by emf measurement ?   5

(c) Calculate the mean activity coefficient of a 0.02 molar aqueous solution of zinc chloride. (Given $A = 0.509$)   5

OR

(a) Derive Lipmann equation.   10

(b) Give the brief discussion of Debye-Huckel limiting law.   5

(c) Explain Stern model of electrified interface.   5

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(4)

Unit-IV

4. (*a*) What are consecutive reactions ? Give the kinetics of consecutive reactions and explain transient equilibrium and secular equilibrium of reactions.   10

   (*b*) What is Salt effect ? Explain the salt effect involved in catalytic reactions ?   5

   (*c*) Give the application of steady state kinetics to the thermal reaction between hydrogen and bromine.   5

OR

   (*a*) What are the postulates of transition state theory ? Derive Eyring equation on the basis of transition state theory.   10

   (*b*) Discuss integral and differential methods of determining rate law.   5

   (*c*) Write a note on Belousov-Zhabotinsky reaction.   5

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