

**D.K.M. COLLEGE FOR WOMEN (AUTONOMOUS), VELLORE-1**  
**ELECTROCHEMISTRY AND QUANTUM CHEMISTRY**

**UNIT-I      Electrochemistry – I**

**SECTION-A (6 Marks)**

1. Describe in detail about the mean ionic activity and mean activity co-efficient.
2. Derive Debye Huckel Bronsted equation .
3. Explain in detail about the Debye huckel limiting law.

**SECTION-B (15 Marks)**

4. Explain in detail about the Debye-Huckel theory of strong electrolytes.
5. Determine the activity and activity co-efficients by electrochemical methods.
6. Describe briefly about the Debye Huckel limiting law with its qualitative and quantitative verification.
7. Describe briefly about the Debye Huckel limiting law at appreciable concentrations of electrolytes.

**UNIT-II      Electrochemistry – II**

**SECTION-A (6 Marks)**

1. What is diffusion? And explain the effect of ionic association on and conductance.
2. What is electrode and electrolyte interface.
3. Explain the lippmann equation.
4. Briefly explain the membrane potential.
5. Define the diffusion and explain the Fick's II law of diffusion.
6. Write a note on electrokinetic phenomena.
7. Write a note on electro capillary phenomena.
8. What is zeta potential?
9. Explain the streaming potential.

10. Discuss the Guoy Chappmann electrical double layer.
11. Explain the stern model of double layer.
12. Explain the Helmholtz perrin model of electrical double layer.

#### **SECTION-B (15 Marks)**

13. Describe the electrical double layers of Helmholtz-perrin and guoy chappmann model.
14. i. Explain the stern model of double layer.(7)  
ii. Explain the Sedimentationa potential.(8)
15. i. Explain the ficks laws of diffusions.(8)  
ii.Briefly explain the electro capillary phenomena. (7)
16. i. Write note on electrokinetic phenomena-membrane potential (10)  
ii. Explain the lippmann equation.(5)

### **UNIT-III Electrochemistry – III**

#### **SECTION-A (6 Marks)**

1. What is polarization and over potential and explain the theories of it.
2. Explain the mechanism of Hydrogen evolution reaction.
3. Explain the mechanism of oxygen evolution reaction.
4. Describe the symmetry factor and its significant.
5. Write a note on corrosion and types of corrosion.
6. Briefly discuss the passivity of metals and how to prevent it.
7. Describe the pourbaix diagram for zinc metal
8. Explain the evans diagram and its application.
9. What is electro deposition and explain the applications.
10. Explain the electrochemical inorganic reactions of technological importance.
11. What is fuel cell and what are all the types of fuels cells.
12. Explain the irreducible current density of the electronation reaction.
13. Explain the symmetry factor and reducible current density of the electron transfer reaction.

### **SECTION-B (15 Marks)**

14. Describe in detail about the Butler-Volmer equation for one step electron transfer reaction and its significance.
15. Write note on
  - i. Corrosion of metal
  - ii. passivity of metals
  - iii. Fuel cells.
16. i. Explain the pourbaix diagram for iron and zinc metal (8).  
ii. Write a note on Evans diagram (7).
17. i. Explain the symmetry factor of one electron transfer reaction. (7)  
ii. Briefly explain the principal of electrodeposition and its applications.(8)

### **UNIT-IV Quantum Chemistry – I**

#### **SECTION-A (6 Marks)**

- 1). Sketch the potential energy curve for simple harmonic oscillator and find out the value of energy when  $V=0$ .
- 2) Explain wave particle duality of electron.
- 3). What is Born- Oppenheimer approximation?
4. Write the Schrodinger equation, radial equation and energy equation of hydrogen atom
5. Discuss about the wave function, significance of wave function and the conditions for acceptable wave functions

#### **SECTION-B (15 Marks)**

- 1)a. Derive the schrodinger equation to a particle in a three dimensional box.  
b. Explain the uncertainty principle.
2. a. Derive the energy and wave function of the particle in one dimentional box.  
b. Explain the radial equation of hydrogen atom.
3. a. Derive the energy and wave function of the particle in the ring.

- b. Explain Compton effect.
- 4. a. Explain about photoelectric effect and black body radiation.
- b. Give the quantum mechanical postulates.
- 5. a. Derive wave function of harmonic oscillator and explain the existence of quantized energy states.
- b. Derive the energy and wave function of rigid rotor.
- 6. a. Explain about the Schrodinger wave equation for hydrogen atom.
- b. Explain about Hermitian operator.
- 7. Account for the following
  - a. Compton effect.
  - b. Wave particle duality.
- c. Uncertainty principle
- 8. a. Explain about the theory of wave motion and derive the Schrodinger wave equation using it. (6)
- b. What is meant by Hermitian operators? Explain and prove the properties of Hermitian operators. (6)
- c. What is photoelectric effect? (3)

### **UNIT-V Quantum Chemistry – II**

- 1. Write notes on perturbation method. How it is applied to Helium atom.
- 2. Explain about SCF.
- 3. Explain about Hartree and Hartree Fock operator.
- 4. Derive the energy and wave function for ethylene molecule using HMO
- 5. Derive the energy and wave function for benzene molecule using HMO
- 6. Explain the VBT theory for hydrogen atom
- 7. Derive the energy and wave function for the diatomic molecules using MOT

### **SECTION-B (15 Marks)**

- 8. a. Apply HMO to ethylene. Obtain the values of energy and function.
- b. Write short notes on Slater type orbital.

9. Derive the energy and wave function of butadiene and explain the stabilization energy.
10. Prove variation method is the best method by applying in helium atom compared with perturbation method.
11. Explain the MOT of hydrogen molecules and ions.
12. Explain the VBT of hydrogen molecule.
13. a. What is perturbation theory? Apply the first order perturbation theory to Helium atom and obtain the expression for its ground state  
b. Derive the ground state energy of hydrogen atom in a.u by variation method
14. a. Write short notes on slater type orbitals.  
b. What is perturbation method? Explain the application of perturbation method for hydrogen and helium atom.  
(3+12)
15. a. Explain about Born-Oppenheimer approximation and derive its expression. (8)  
b. Explain about HF-SCF method. (7)
16. a. Derive an expression for Huckel theory for conjugated molecule benzene. (8)  
b. Explain about semi empirical methods. (7)