

SHRIMATHI DEVKUNVAR NANALAL BHATT VAISHNAV COLLEGE FOR WOMEN
(AUTONOMOUS)

(Affiliated to the University of Madras and Re-accredited with 'A+' Grade by NAAC)
Chromepet, Chennai - 600 044.

M.Sc.Chemistry - END SEMESTER EXAMINATIONS - NOV' 2024

SEMESTER - III

22PCHCT3009 - Electro and Computational Chemistry

Total Duration : 2 Hrs. 30 Mins.

Total Marks : 60

Section B

Answer any **SIX** questions ($6 \times 5 = 30$ Marks)

1. Give an account of the Debye-Huckel theory of strong electrolytes.
2. Explain the electro kinetic phenomena with the concept of forces and flux.
3. Outline the applications of over potential.
4. Describe the working principle of electrode deposition.
5. What are the applications of the Guassian software? Explain with an example.
6. Illustrate the electro kinetic phenomenon and zeta potential.
7. Outline the mechanism of discharge and recharge process of a secondary battery.
8. Calculate the mean activity coefficient γ_{\pm} of NaCl at a molality of 0.01 in aqueous solution at 25°C.

Section C

I - Answer any **TWO** questions ($2 \times 10 = 20$ Marks)

9. (a) Derive the Debye-Huckel limiting law equation.
(b) Derive the Debye-Huckel limiting law equation and discuss its validity.
10. Describe the applications of density functional theory.
11. Derive Butler Volmer equation for one electron transfer reactions.
12. Highlighting the causes and consequences of corrosion illustrate the cathodic and anodic prevention.

II - Compulsory question ($1 \times 10 = 10$ Marks)

13. Compare the double layer theories of Helmholtz-Perrin, Guoy Chapmann and Stern models.
