

Roll.No.

25PCHCT3009

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 - NOVEMBER 2025
SEMESTER - III

25PCHCT3009 - 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. Explain the concept of ionic strength. Calculate the ionic strength of a solution containing 0.02 M $MgCl_2$ and 0.01 M Na_2SO_4 .
2. Derive the Butler–Volmer equation for a one-electron transfer reaction and explain its limiting cases
3. Evaluate the effectiveness of cathodic protection versus anodic inhibitors in preventing corrosion of underground iron pipelines. Support your answer with reference to Evans diagrams.
4. How can molecular mechanics be applied to predict the stable conformation of n-butane? Mention the energy terms involved in the force field.
5. Describe the Helmholtz–Perrin model of the electrical double layer. How does it differ from the Gouy–Chapman model in terms of charge distribution?
6. Analyze why the Tafel slope for hydrogen evolution on mercury is ~ 120 mV/dec, while on platinum it is ~ 30 mV/dec. Relate your answer to the mechanism (Volmer–Heyrovsky vs. Volmer–Tafel) and exchange current density.
7. Using the $Fe - H_2O$ Pourbaix diagram, analyze the regions of immunity, corrosion, and passivation of iron at $pH = 2$ and $E = -0.6$ V vs SHE.
8. Why is Density Functional Theory (DFT) preferred over Hartree–Fock for studying transition metal complexes? Evaluate based on electron correlation and computational cost.

Section C

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

9. Derive the Debye–Hückel limiting law and discuss its significance.
10. Compare the Stern model with the Gouy–Chapman model in explaining the capacitance behavior of the electrical double layer at high electrolyte concentrations.

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11. Explain the mechanism of electrode reactions, polarization, and overpotential with suitable examples.
12. Create an optimal design for a secondary battery for electric vehicles by evaluating energy density, cycle life, safety, and cost of Li-ion, Ni–Cd, and lead–acid systems. Recommend one with justification.

II - Compulsory question (1 × 10 = 10 Marks)

13. Discuss the Debye Huckel theory of strong electrolytes.
