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 - 2023
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. Calculate the Debye-Huckel limiting law constant (A) for a solution with an ionic strength of 0.05 M at $25°$C.
2. Compute the ionic strength of a solution containing 0.1 M NaCl and 0.2 $MKNO_3$.
3. Predict the capacitance of an electrochemical double layer formed at a platinum electrode immersed in 0.1 M NaCl solution at $25°$C. Assume the Stern model applies, and the surface area of the electrode is $110_{-3}\ m^2$.
4. Give the significance of equilibrium exchange current density, symmetry factor and transfer co-efficient.
5. Compare primary and secondary batteries with examples.
6. Calculate the maximum electrical work (in joules) for a silver-zinc cell (has a theoretical voltage of 1.65 V) that can be obtained from this cell when it discharges completely.
7. Discuss basis sets and its types.
8. Write the Z-matrix for the ethane and ethylene.

Section C

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

9. Derive and verify Debye Huckel Onsager equation.
10. Discuss the Helmholtz-Perrin, Guoy Chapmann and Stern models of electrical double layers.
11. Deduce Butler Volmer equation for one-electron transfer reactions.
12. Discuss various theories of corrosion and prevention of corrosion by any two methods.

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

13. Determine the electronic energies using Hartree -Fock calculations for a molecule.

******