**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-600 **Title of the course:** Practical Course in Physical Chemistry - III

**Number of Credits:** 4

**Effective from AY:** 2023-24

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| **Prerequisites for the course:** | Should have studied Physical chemistry practical course at M.Sc. Part-I. | |
| **Course Objectives:** | 1. To introduce concepts of Kinetics and Thermodynamics<br>2. To introduce concepts of Surface science and Catalysis<br>3. To introduce various concepts of Electrochemistry<br>4. Introduction to the use of computers and computational tools in chemistry | |
| **Contents** | *Note: A minimum of 7 experiments from each Unit I-III are to be completed.*<br>**Unit - I. Instrumental**<br>a. To determine the redox potential of $Fe^{2+}/Fe^{3+}$ system using rotating disk voltammetry method.<br>b. To determine the instability constant of the reaction $[Ag(NH_3)_2]$----> $Ag + 2NH_3$ potentiometrically.<br>c. To determine the transport number of ions using moving boundary method.<br>d. To verify Nernst equation and determine the standard oxidation potential of copper and zinc electrodes.<br>e. To study effect of ionic strength on activity coefficient of $Ag^+$ ions.<br>f. To investigate the reaction kinetics between Potassium Persulphate and Potassium Iodide colorimetrically.<br>g. To determine the equivalent conductance of a strong electrolyte (KCl) at several concentrations and verify Onsager's equation.<br>h. To estimate the concentration of Sulphuric acid, Acetic acid and Copper sulphate in a given solution conductometrically.<br>i. To determine the concentration of $Fe^{2+}$ ions by titrating with potassium dichromate conductometrically.<br>j. To study the kinetics of hydrolysis of tertiary butyl chloride by conductometry.<br>k. To determine the half wave potential of $Cu^{2+}/Cd^{2+}/Zn^{2+}$ by using polarography.<br>l. To study the effect of sol-gel and hydrothermal method of synthesis on crystallite size and surface area of a semiconductor catalyst.<br>m. To investigate the effect of catalyst loading on photocatalytic degradation of azo dye using semiconductor catalyst.<br>n. To study the stress-strain response of polymeric materials and compare their strength. | No of hours<br><br>40 |

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| | o. To determine the degradation rate of the polymers using thermogravimetric methods.<br>p. To determine the curie temperature of conducting polymer samples.<br>q. To determine the resistivity of polymeric material using four probe method. | |
| | **Unit - II. Non-Instrumental**<br>a. To determine the critical micelle concentration of three types of surfactants using stalagmometer.<br>b. To determine the partial molal volume of sodium chloride-water, ethanol-water and methanol-water system by apparent molal volume method.<br>c. To study the effect of surfactants on surface tension of water using stalagmometer.<br>d. To study the variation of viscosity with composition of mixtures and to verify the formation of compounds by Oswald's viscometer.<br>e. To study the effect of pH on the kinetics of iodination of Aniline.<br>f. To study the kinetics of reaction between $H_2O_2$ and KI (clock reaction).<br>g. To study the kinetics of rapid reaction between Bromine and Iodine in aqueous media.<br>h. To investigate the autocatalytic reaction between Potassium Permanganate and Oxalic acid.<br>i. To study the electroless deposition of Ni on non-conductor substrate and to determine the rate of deposition.<br>j. To study the variation in catalytic activity of three different metal oxides for $H_2O_2$ decomposition reaction.<br>k. To investigate the effect of pH on adsorptive separation of azodye from water using MCM-41. | 40 |
| | **Unit - 3. Computational Chemistry**<br>a. To generate a mark sheet and understand various features of spreadsheets.<br>b. To generate a plot for a given function such as solutions of 1D box, harmonic oscillator, H-like atom wave functions, Gaussians distributions etc.<br>c. To write a computer program to obtain equivalence point in pH metry and potentiometric experiments (derivative method).<br>d. To write a computer program to find percent composition for various atoms of a given molecular formula.<br>e. To write a computer program to obtain slope and intercept for linear data using least square fit method.<br>f. To write a computer program to obtain center of mass of a given molecule and moment of inertia, hence obtain classification of the | 40 |

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| | given molecule.<br>g. To write a computer program to find out various parameters for data analysis viz. minimum, maximum, average, standard deviation, variance, covariance, correlation coefficient, frequency distribution etc.<br>h. To write a computer program to obtain thermodynamic probability.<br>i. To write a computer program to obtain degeneracy of a given energy level for a particle in a cube.<br>j. Calculate the ground state energy of hydrogen atom using various basis sets using *ab-initio* program.<br>k. Calculate and interpret the IR, RAMAN and NMR spectra of simple organic molecules using *ab-initio* program. | |
| **Pedagogy:** | Mainly pre-labs / practicals or a combination of some of these could also be used to some extent. | |
| **References / Readings:** | 1. A. Finlay and J.A. Kitchener, Practical Physical Chemistry, Longman Publisher, 1963.<br>2. A. M. James, Practical Physical Chemistry, Longman Publisher, 1974.<br>3. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGraw-Hil, 1981.<br>4. J. B. Yadav, Advance Practical Physical Chemistry, Krishna Educational Publishers, 2014.<br>5. S.Attila, and N. S. Ostlund. Modern quantum chemistry: introduction to advanced electronic structure theory. Courier Corporation, 2012.<br>6. P.P. Morajkar, A. P. Naik, S. T. Bugde, B. R. Naik, CH-20: Photocatalytic and microbial degradation of Amaranth dye, Advances in Biological Science Research-A Practical Approach 2019, 327-345, Academic Press.<br>7. J.B. Foresman, E. Frisch, Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian, 2nd Ed. Gaussian, 1996 | |
| **Course Outcomes:** | 1. Student should be able to apply the concepts of physical chemistry in M.Sc. Dissertations.<br>2. Students shall be equipped with practical skills needed for research and development.<br>3. Students will understand the instrumental and non-instrumental methods of analysis.<br>4. Students will understand use of computers and computational tools in chemistry. | |