## SYLLABUS OF COURSEWORK FOR DOCTOR OF PHYLOSOPHY

Ph.D. (Science)
Subject: Chemistry
(Under Faculty Council of Science)

2019



# Department of Chemistry Diamond Harbour Women's University Sarisha, West Bengal 743368.

(Revised on 18/03/22 and Effective from the Academic Session 2022-23)

#### SYLLABUS OF Ph.D. (Sc.) COURSE WORK

## Department of Chemistry DIAMOND HARBOUR WOMEN'S UNIVERSITY

- Duration : One Semester (6 Months)
- Total Marks: 200 (Two papers 100 marks each, 4 credit point each)
- Duration of Examination: 4 Hrs. (2 Hrs. for each paper)
- Compulsory Units: Research Methodology & Review of Research Work: 100 Marks (4 credits, 2 hrs)
- Elective Units: Subject Course Work: 100 Marks (4 Credits, 2 hrs. each)

Paper Code	Paper Name	Full Marks	Periods/Week
CHEM/PhD/CP/01	Research Methodology	50	02
CHEM/PhD/CP/02	Review of research work and Presentation	50	02
CHEM/PhD/EP/01	Elective Paper	50	02
CHEM/PhD/EP/02	Elective Paper	50	02
Total=		200	08

Compulsory Papers: CHEM/PhD/CP/01 & CHEM/PhD/CP/02

**Elective Paper**: Students have to choose **four** Elective units (**maximum three units from any one group**) from the following list which will be offered by the department, depending on students interest and availability of expertise.

#### **Elective Paper:**

CHEM/PhD/EP/01: i) First unit from any one of I.1., O.1 & P.1; ii) Second unit from any one of I.2., O.2 & P.2. (Total 50 Marks, 25 from each unit)

CHEM/PhD/EP/02: i) First unit from any one of I.3., O.3 & P.3; and ii) Second unit from any one of I.4., O.4 & P.4. (Total 50 Marks, 25 from each unit)

#### **Elective Units:**

Group A:	Group B	Group C		
I.1. Single Crystal X-	O.1. Synthetic Methodology	P.1. Theoretical Chemistry		
Ray Structures,		•		
Supramolecular				
Chemistry.				
I.2. Materials, Catalyses	O. 2. Applied chemistry	P.2. Chemical and Electrochemical		
and Electrochemical		Kinetics and Environment		
Studies.		Related Electrochemistry		
1016.1.1.1.6	0.2 Pi	,		
I.3 Metals in Life.	O.3. Bio-organic Chemistry	P.3. Biophysical Chemistry and		
		Surface Chemistry		
I.4. Application of	O.4. Spectroscopy	P.4. Photochemistry and		
Spectroscopic Studies in	and Asymmetric	Spectroscopy		
Chemical Research.	Synthesis			
<b>16X4</b> classes to be attended.				

#### **Nomenclature of Compulsory Unit:**

Illustration: I.2 Abbreviations: I: Inorganic Similarly O: Organic; P: Physical] & the digit represents Unit No.

### Ph.D. Course Work in Chemistry (Compulsory Papers)

Paper Code: CHEM/PhD/CP/01 Paper Name: Research Methodology

- **1. Scientific Research:** Research: Definition, Characteristics, types, need of research. Identification of the problem, assessing the status of the problem, formulating the objectives, preparing design (experimental or otherwise), Actual investigation, Determining the mode of attack.
- **2. Literature survey:** References, Abstraction of a research paper, Possible ways of searching of current literature.
- **3. Documentation and scientific writing:** Results and Conclusions, Preparation of manuscript for Publication of Research paper, Presenting a paper in scientific seminar. Thesis writing, Structure and Components of Research Report, Types of Report: Research Papers, Thesis, Research Project Reports, Pictures and Graphs, Citation styles, Writing a review of paper, Bibliography.
- **4. Computer fundamentals:** Basic idea of computer fundamentals, Different operating systems, Uses of word processing software- MS Word/Latex/others, Drawing graphs and diagrams using—Origin/Excel/gnuplot/others. Computer usage for collecting/analyzing data— simulations using Fortran/C/Mathematica/Matlab/others. Preparing presentations—Power point for oral and poster presentations
- **5.** Use of internet in research works Use of internet networks in research activities in searching material, paper downloading and submission in arXives, use of SPIRES database, relevant websites for journals and arXives.
- **6. Introduction to Patent laws etc.** Patent laws, process of patenting a research finding, Copy right, Cyber laws.

Ph.D. Course Work in Chemistry
(Compulsory Papers)
Paper Code: CHEM/PhD/CP/02
Paper Name: Review Work and Presentation

Review work is to be focused on the essential content of any three papers or review articles in her area of interest. The relevance of research from perspective of the subject, detailed review and scope of the work are to be reviewed. A presentation will have to be delivered by the research scholar at the end of the semester along with a synopsis/report of her review work.

## Ph.D. Course Work in Chemistry (Elective Units)

#### **Group-A (Inorganic Chemistry)**

#### Unit-I.1: Single Crystal X-Ray Structures, Supramolecular Chemistry

Crystal growth and data collection; Structure solution and refinement; Supramolecular Chemistry.

#### Unit-I.2: Materials, Catalyses and Electrochemical Studies

Homogeneous and Heterogeneous catalysis; Polarog,raphy; Potentiometry; Amperometry, Coulometry, Voltametry.

#### **Unit-I.3: Metals in Life**

Environmental health-hazards and remediation; Metalloproteins; metalloenzymes; photosystem; DNA interaction.

#### Unit-I.4: Application of Spectroscopic Studies in Chemical Research

IR and UV-Visible Spectroscopy; Luminescence Spectral Studies; Mass Spectrometry; NMR and ESR Spectrometric application; CD and ORD treatment.

#### **Group-B** (Organic Chemistry)

#### **Unit-O.1: Synthetic Methodology**

Organometallic Chemistry; Boron-, Silicon-, Phosphorus Chemistry, Green Chemistry

#### **Unit-O.2: Applied chemistry:**

Polymer, Composites, Nano composites, Bio composites, Surface modification of Materials and its techniques. Thermal and Rheological properties of polymers and composites.

#### **Unit-O.3: Bio-organic Chemistry**

Biomimetics; nucleoside-, nucleotide-chemistry; Small molecule and DNA interaction, Bioconjugation chemistry.

#### **Unit-O.4: Spectroscopy and Asymmetric Synthesis**

<sup>1</sup>H, <sup>13</sup>C, 2D & other nuclei; Mass Spectrometry; Asymmetric Synthesis.

#### **Group-C** (Physical Chemistry)

#### **Unit-P.1: Theoretical Chemistry**

#### **Basic Quantum Mechanics**

A review of Schrödinger formulation; One-dimensional potential barrier problems; Schrödinger, Heisenberg and Interaction problems; Variation and perturbation methods; Time-dependent perturbation; applications.

#### Statistical Mechanics and Computer Simulation

An introductory review of Statistical Mechanics (Real gas, Monatomic Liquids); Introduction to the time correlation function formalism (Absorption of Radiation, Classical theory of light scattering); Computer Simulation Techniques.

#### Irreversible Thermodynamics

Internal heat and entropy production; Relation of entropy production with Fluxes & Forces; Phenomenological equation; Onsager reciprocal relation; Prigogine's principle of minimum entropy production at non equilibrium stationary state.

#### Unit-P.2: Chemical and Electrochemical Kinetics and Environment Related Electrochemistry

Fuel cells; Solar cells (photochemical, photovoltaic); Batteries (solid-state & conventional)-single electrode and complete cell studies; Production of  $H_2$  and important chemicals of high energy; Corrosion & waste removal techniques.

#### Electrochemical Techniques

Polarog, raphy; Chronopotentiometry; Chronoamperometry, Chronocoulometry, Linear Potential Sweep Voltametry; Cyclic Voltametry, Impedance measurements; AC Voltametry.

#### **Reaction Dynamics**

Factors affecting the chemical reaction rate: temperature, ionic strength of the solution, catalyst, pH and dielectric constant of the medium, micelle, reverse micelle & nanoparticles; Determination of rate constant by stopped flow method & relaxation method; Flash photolysis & use of LASER

#### **Unit-P.3: Biophysical Chemistry and Surface Chemistry**

Thermodynamics in Biochemistry (Fundamentals and Applications); Biopolymers (Proteins, Enzymes, DNA, Carbohydrates); Biomembranes (Structure and Function); Active

transport and passive transport, Multiple equilibria, Specific examples of multiple equilibria, Transport processes; General features of transport processes; Optical systems for the study of transport processes, Self organizing systems (Micelles, Lipids. Cyclodextrins, Liquid crystals, Reverse micelles, coacervates, Proteins *etc*) their interactions and solutions properties.

Preparation, Characterization and Application of nanoparticles

Surface and Biophysical Techniques: CD, SEM, TEM, EDAX, DLS, Gel Electrophoresis, Radioactivity, XPS.

#### **Unit-P.4: Photochemistry and Spectroscopy**

Photon molecule interactions; Absorption, fluorescence and phosphorescence; Quantum yield; Non- radiative deactivations; Excited state; Phosphorescence; Steady state and time resolved aspects; Time-resolved Fluorescence; Flash photolysis; Types of photochemical reactions; Change of properties of molecules upon photo excitation; Photoelectron Spectroscopy; Mossbauer Spectroscopy; Raman Spectroscopy. Selection rules in spectroscopy, Fermi resonance, electronic spectroscopy, progression and sequences, introduction to laser spectroscopy, synthesis of cold molecular clusters.