FACULTY OF PHYSICAL SCIENCES

REVISED SYLLABI

FOR Ph. D. CHEMISTRY COURSE WORK
(SEMESTER SYSTEM)
(SESSION 2019-20 AND ONWARDS)

HIMACHAL PRADESH UNIVERSITY
DEPARTMENT OF CHEMISTRY, SHIMLA-171005
INDIA
Annexure-“C”
A Detailed Scheme and Course Contents of the Syllabi for PhD . Chemistry Spread Over two Semesters (I-II)
For Session 2019-20 and Onwards

**SEMMESTER-I**

Each candidate has to study three papers in first semester. Paper I (Research Methodology) is compulsory paper and two papers (optional Paper-II and III) from the respective specialization i.e. Inorganic Chemistry, or Organic Chemistry or Physical Chemistry. Each paper will be of 100 marks.

<table>
<thead>
<tr>
<th>Paper No.</th>
<th>Title</th>
<th>Max. Marks</th>
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<tbody>
<tr>
<td>Paper 1</td>
<td>Research Methodology</td>
<td>100</td>
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<tr>
<td></td>
<td>(Compulsory for all specialization)</td>
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<tr>
<td></td>
<td><strong>Inorganic Chemistry</strong></td>
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<tr>
<td>Paper -II</td>
<td>Inorganic Chemistry (Advanced Inorganic Chemistry)</td>
<td>100</td>
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<tr>
<td>Paper -III</td>
<td>Inorganic Chemistry (Inorganic and Superamolecular Chemistry)</td>
<td>100</td>
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<tr>
<td></td>
<td><strong>Organic Chemistry</strong></td>
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<tr>
<td>Paper -II</td>
<td>Organic Chemistry (Organic Synthesis)</td>
<td>100</td>
</tr>
<tr>
<td>Paper -III</td>
<td>Organic Chemistry (Polymer Chemistry)</td>
<td>100</td>
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<td></td>
<td><strong>Physical Chemistry</strong></td>
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<tr>
<td>Paper -II</td>
<td>Physical Chemistry (Kinetics of Fast Reactions and Advanced Electrochemistry)</td>
<td>100</td>
</tr>
<tr>
<td>Paper -III</td>
<td>Physical Chemistry (Non-Equilibrium Physical Chemistry and Theoretical and Applied Aspects of Surfactant System)</td>
<td>100</td>
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Semester 1  
M.Phil. Chemistry  
Paper-I (Research Methodology)  

Lectures: 60  
Max. Marks: 100  

Note: Examiner will set 10 questions, two from each section and the candidates will be required to attempt five questions in all selecting at least one question from each section. All questions will carry equal marks.

Section A  
Research Methodology: Types and methods of research, classification of research, pure and applied research, exploring or formulative research, descriptive research, diagnostic research/study, Evaluation of research/study, action research, and experimental research-problem selection. Meaning, Scope, Primary sources of literature survey, Journals, patents etc., secondary sources of literature survey, Books, Reference books, Text books, listing of letters.

Section B  

Section C  
Concepts of chemical safety: Chemical safety and ethical handling of chemicals, safe working procedure and protective environment, emergency procedure and first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmosphere, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals.

Section D  
Research ethics: Ethical issues, copy right, royalty, intellectual property rights, citation and acknowledgement. Reproducibility. Safety rules of laboratory acquaintance of experimental set up, importance of safety and security of data. Review of published research in the relevant field, training, field work.

Section E  
Computer applications in research: Application and uses of common softwares in chemistry-origin, chemsketch, chemdraw, basic ideas on the use of internet in chemistry education.

Reference Books:  
11. Research Methodology. Methods and Techniques : C. R. Kothari,
NOTE: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

UNIT-I
Catalysis Involving Organometallic compounds: Homogeneous hydrogenation and hydroformylation of unsaturated compounds (Olefins). Hydroformylation, hydroisilylation of unsaturated compounds, hydrocyanation of alkenes; alkenes and alkynes metathesis.

UNIT-II
Co-ordination Addition Polymerisation: Zeigler Natta catalysts, composition, nature and mechanism of stereo specific placement in polymerisation, bimetallic and monometallic mechanism, stereoregulation. Supported metal oxide catalysts, polymerisation mechanism, bound-ion radical mechanism and bound-ion co-ordination mechanism. Metallocene based Zeigler Natta catalysts, catalysts composition, active centre and polymerisation mechanism.

UNIT-III
Synthesis of Coordination compounds: Theoretical consideration: Labile and Inert Coordination compounds, synthesis of mixed ligand complexes by co-propotionation, chelate effect, trans effect (Peyrone’s rule, Jorgenson’s rule and Kurnakov’s rule), Cis effect. Geometric isomerization of square planer platinum(II) and Palladium(II) complexes, hard-soft acid-base (HSAB) principle, factors affecting the acid base properties of coordination compounds, ligand effects on redox potentials of coordination compounds.

UNIT-IV
Voltammetric methods of analysis: Principle, excitation signals, mass transfer mechanism, instrumentation, methods of analysis and applications of pulse polarography, cyclic voltammetry and anode stripping voltammetry. Use of cyclic voltammetry for the determination of formal reduction potential and number of electron change for ferri/ferrocyanide couple and to study electrode mechanisms of electron reduction of nitrobenzene and voltammetry with microelectrodes.

UNIT-V

Books Recommended:
1. Homogeneous transition metal catalysis – Christopher Masters
2. Principles and Application of Homogeneous Catalysis – Nakamura and Tsutsui
3. Advanced Polymer Chemistry- Manas Chanda
5. Fundamentals of Analytical Chemistry- Skoog, West, Holler and Crouch
6. Chemistry experiments for Instrumental methods- Sawyer, Heineman and Beebe.
9. Principles and applications of organotransition metal chemistry by Ccollim and Hegden
Semester 1
M.Phil. (Inorganic Chemistry)
PAPER – III (Inorganic and Superamolucular Chemistry)

Lectures: 60
Max. Marks: 100

NOTE: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

UNIT-I
a) **Role of Metal-ions in Biological Systems**: Metal-ion-interactions with Nucleosides and Nucleotides, Metal-ion-interactions with DNA, Metal-ion-interactions with RNA.

b) **Electron-Transfer Agents in Biological Systems**: Cytochromes, Iron sulphur proteins, Vitamin B₁₂ and B₁₂ Coenzymes Xanthane oxidase, Superoxide dismutase.

UNIT-II
a) **Supramolecular Reactions and Catalysis**: Introduction, Catalysis by reactive macrocyclic cation receptor molecule, by reactive macrocyclic anion receptor molecule Supramolecular metallocatalysis.

b) **Supramolecular Assemblies**: Introduction, Supramolecular solid materials, Molecular recognition at surfaces (Endoreceptors vs Exoreceptors), Molecular and Supramolecular Devices, Photonic, electronic and Ionic Devices.

UNIT-III
**Reactions at Coordinated Ligands**: Reactions due to metal ion polarization of co-ordinated ligands, Aldol Condensation, Imine formation, hydrolysis and substituent exchange. Template effect and macrocyclic ligands.

UNIT-IV

UNIT-V

Books Recommended:
2. Inorganic Chemistry - Purcell and Kotz.
3. The Inorganic Chemistry of Biological Process-M.N. Hughes (2nd Edn.)
5. Inorganic Reaction Mechanism - Bassolo and Pearson.
Semester 1
M.Phil. (Organic Chemistry)
PAPER – II (Organic Synthesis)

Lectures: 60
Max. Marks: 100

NOTE: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

UNIT – I
Spectroscopy: Basic theory, Instrumentation and applications of UV spectroscopy, IR Spectroscopy, NMR Spectroscopy and Mass spectrometry in organic compounds. Problems based on IR, UV, NMR and mass spectral data.

UNIT - II

Reagents in Organic Synthesis: Reagents in organic synthesis: Willkinson catalyst, Triphenylphosphine-alkyl halid reagent, Lithium dialkyl cuprates (Gilman’s reagents), Lithium disopropylamid (LDA), Dicyclohexylcarbo dibimide (DCC), and Tri-n-butyltinhydride. Nickel tetracarbonyl, Trimethylchlorosilane.

UNIT–III


UNIT–IV
Stereochemistry: Stereoselective and stereospecific reactions: Stereoselective reactions: Hydride reduction of cyclic ketones, catalytic hydrogenation, Stereoselective nucleophilic addition to acyclic carbonyl groups stereospecific reactions: Bromination of alkene, Epoxidation and dihydroxylation of alkenes, Hydroboration oxidation. Analysis and separation of enantiomeric mixture:

Chiral shift reagent and chiral solvating agents, Separation of enantiomers by chromatography. Enzymatic separation and desymmetrization using lipases, proteases, Acylases and epoxide hydrolases.

UNIT–V

Books Recommended:
10. Organic Synthesis: Jagmohan Singh and Yadav
15. Introduction to Medicinal Chemistry, Alex Gringuage.
Semester 1
M.Phil. (Organic Chemistry)
PAPER – III (POLYMER CHEMISTRY)

Lectures: 60
Max. Marks: 100

NOTE: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

UNIT-I
Polymer Synthesis: Kinetic and mechanism of radical, cationic, and anionic addition polymerization, Living polymerization. Significance of chain transfer reactions, Chemistry and kinetics of inhibition and retardation. Miscellaneous polymerization reactions: Monomers with two different polymerizable groups, Hydrogen transfer polymerization, Polymerization and cyclotrimerization of isocyanates, Monomers with triple bonds, Ring opening polymerization: Scope, polymerizability, polymerization mechanism and kinetics, examples of cyclic amide and ethers; Monomers containing the same functional groups, Monomers containing different functional groups, Zwitterionic copolymerization.

UNIT –II

UNIT- III
Polymer Characterization: Determination of molecular weight of polymers by colligative properties, viscosity measurement, end group analysis, sedimentation velocity and equilibrium method. Analysis and Characterization of polymers by chemical analysis, FTIR, NMR, TGA, GPC, DSC, XRD, SEM techniques.

UNIT- IV
Special Polymer Reactions: General introduction to the polymer reactions, Derivatization reactions of biopolymers – cellulose, chitosan, starch and natural gums. Polymer as carriers or supports, polymeric reagents, polymeric substrates, polymeric catalysts, immobilized enzymes. Polymer stability and degradation: Type of degradation, mechanism, ultrasonic, photo, high energy and oxidative degradation, Fire retardants, UV stabilizers and absorbers. Biodegradation by alkali, acid, ionic liquids and enzymes, hydrolytic reactions of biopolymers and their special technological potential with respect to bio-ethanol.

UNIT-V

Books Recommended
NOTE: Ten questions will be set by the examiner selecting TWO from each unit and every question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

Kinetics of Fast Reactions

UNIT I
Basic Principles of Chemical Relaxation Techniques: Relaxation time and its significance, determination of rate constants from relaxation data. Evaluation of relaxation time form a relaxation oscillogram. Relaxation time in multi step systems. Chemical relaxation in two and multi step systems. Thermodynamic aspects in relation to chemical relaxation; Gibbs free energy, affinity of a reaction and advancement of a reaction.

UNIT II
Experimental Techniques for the Study of Relaxation Kinetics (Theory and Applications):
- Pressure Jump Technique: Application to mechanistic investigation of relaxation behaviour in Beryllium Sulphate solution and determination of thermodynamic quantities from amplitude data of relaxation oscillogram.
- Temperature Jump Technique: Application to mechanism of water addition to carbonyl functional group of organic carbonyl compounds.
- Electric Field Jump Technique: Application to neutralization reaction.

Advanced Electrochemistry

UNIT III

UNIT IV

UNIT V
Surface Electrochemistry: The electrified interface, introduction and basic facts of electrocapillarity, thermodynamics of the electrocapillary effect. Thermodynamic treatment of polarizable interface, determination of charge density on the electrode (Lippmann equation), determination of surface excess (variation of surface tension with solvent composition of electrochemical system). The structure of electrified surfaces. The Helmholtz – Perrin theory, the Gouy – Chapman Diffuse – Charge Model of double layer and Stern Model.

Books Recommended:
2. Physical Chemistry of Surfaces: A.W. Adamson
3. Electrochemistry: S. Glasstone
Semester 1

M.Phil. (Physical Chemistry)

PAPER – III (Non – equilibrium Physical Chemistry and Theoretical and Applied Aspects of Surfactant System)

Lectures: 60
Max. Marks: 100

NOTE: Ten questions will be set by the examiner selecting TWO from each unit. Each question will be subdivided into two to three parts. The students shall attempt FIVE questions selecting ONE from each unit.

UNIT – I

UNIT – II
Non Linear Steady States: Non – linear flux equations in respect of electro – kinetic phenomena (expressions as well as some qualitative insight to some experimental results). Non – linear flux equation and non – linear steady state in chemical reactions (i) linear (rate) and non linear flux equation for a single reversible reaction and (ii) linear phenomenological relation and non – linear flux equation for coupled reactions.

UNIT – III
Micelle formation, critical micelle concentration, monodisperse micelles of ionic and non – ionic surfactants and thermodynamics of micelle formation (Mass Action Model). Counterion binding to micelles (Evan and Ninham model). Kinetics of micelle formation. Effect of temperature and pressure on micelle formation (a qualitative treatment). Micelle Temperature Range (MTR) or Kraft phenomenon, physicochemical meaning of MTR and effect of salt on MTR.

UNIT – IV

UNIT – V
Micellar Catalysis and Photochemistry of Micellar System: Effect of micelles on chemical reactions, micelle catalyzed reactions, distribution of reactants among micelles: Poisson and Gaussian distributions. Inhibition in micellar solutions. Determination of CMC by fluorescence probe method (Qualitative view) and micellar aggregation number by fluorescence probe method (Static and dynamic methods).

Books Recommended:
1. Introduction to Non – Equilibrium Physical Chemistry: R.P. Rastogi
5. Micelles (Theoretical and Applied Aspects): Y. Moroi
6. Non – equilibrium Thermodynamics: C. Kalidas
7. Non – equilibrium Thermodynamics: I. Prigogene