

FACULTY OF SCIENCES

SYLLABUS

for

PRE-Ph.D COURSE IN CHEMISTRY

(Credit Based Evaluation & Grading System)

(SEMESTER SYSTEM)

Examinations: 2019-20



GURU NANAK DEV UNIVERSITY

AMRITSAR

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Pre Ph.D. Course in Chemistry (CBE & GS)

Scheme

Code	Paper	Credits
CYL 901	Biocatalysis, Organocatalysis and Inorganic Catalysis	3-0-0
CYL902	Biophysical Chemistry	3-0-0
CYL903	Supramolecular Chemistry	3-0-0
CYL 904	Research Methodology	4-0-0
	Elective course from other departments (Candidate has to choose any one out the below mentioned)	
	ESL964 Good Laboratory Practices	3-0-0
	PHL902 Experimental Techniques	3-0-0
	ESL961 Disaster Management	3-0-0
CYP901	Seminar (Audit Course)	0-0-1

**BIOCATALYSIS, ORGANOCATALYSIS AND INORGANIC CATALYSIS
CYL 901**

Credits: 3-0-0

(45hrs.)

Mid Semester Examination: 20% weightage

End Semester Examination: 80% weightage

Instructions for the Paper Setters:

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

Section A

Biocatalysis in Organic Chemistry: Introduction to Biocatalysis. Application of Biocatalysts: Hydrolytic reactions, mechanistic and kinetic aspects, hydrolysis of amide bond, ester hydrolysis, hydrolysis and formation of phosphate esters, hydrolysis of epoxides, hydrolysis of nitriles. Reduction reactions: recycling of cofactors, reduction of aldehydes, ketones and carbon-carbon double bonds with whole cells. Oxidation reactions : oxidation of alcohols and aldehydes; oxygenation reactions, hydroxylation of alkanes and aromatic compounds, epoxidation of alkene, sulfoxidation reactions, formation of peroxides, dihydroxylation of aromatic compounds; peroxidation reactions. Enzymes in organicsolvents: ester synthesis, lactone synthesis, amide synthesis, peptide synthesis, peracid synthesis, redox reactions, medium engineering. (Books1,2,3)

(12h)

Section B

Organocatalysis in Organic Synthesis: Introduction Enamine catalysis: Aldol and Mannich type reactions, -heteroatom functionalization, direct conjugate additions via enamine activation. Iminium catalysis: the catalysis concept, cycloaddition reactions, 1,4-addition reactions, transfer hydrogen, cascaderactions. Ammonium ions as chiral templates: Homogeneous catalysis with chiral quaternary ammonium salts, Heterogeneous catalysis- chiral phase transfer catalysis. Morita-Baylis-Hillman reaction: addition of ketones and aldehydes to activated olefins, asymmetric MBH reactions. Asymmetric proton catalysis: conjugate addition reactions, hydrocyanation reactions, mannich reactions, aza-henry reaction, acyl Pictet-Spengler reaction, aza Friedel-Crafts reaction. (4,5,6)

(11h)

Section C

Organocatalysis in Organic Synthesis: Chiral Lewis bases as catalysts: allylation reactions, propargylation reactions, hydrocyanation andisonitrile addition, aldol type reactions, reduction of imines, epoxide ring opening. Asymmetric acyl transfer reactions. Nucleophilic N-Heterocyclic carbenes. Ylide based reactions. Organocatalytic oxidation and reduction reactions. (4,5,6)

(6h)

Inorganic Catalysis: *Fundamental reaction steps of transition metal catalysed reaction.* Coordinative unsaturation, oxidative-addition, reductive elimination reactions, migratory insertion and elimination reactions. cleavage of C-H bonds, nucleophilic and electrophilic addition and abstraction.

(7h)

Section D

Inorganic Catalysis: *Homogeneous and heterogeneous catalysis using transition metal complexes.* Catalytic hydrocyanation, hydrosilylation and hydroboration reactions of olefins. alkene isomerization, Hydroformylation reaction of unsaturated compounds, carbonylation reactions: Reppe carbonylation. Olefin metathesis: synthesis of Grubbs and Schrock catalysts, mechanism of olefin metathesis, C-C cross coupling reactions, Olefin oligomerization and polymerization using metallocene and post metallocene based catalysts, oligomerisation using SHOP. Fischer-Tropsch reactions and water gas shift reaction.

(11h)**Books:**

1. Biotransformations In Organic Chemistry: A Textbook by Kurt Faber 5th Edition Publisher: Springer-Verlag, New York, **2009**.
2. Biocatalysis. Fundamentals and Applications by A. S. Bommarium (Georgia Institute of Technology) and B. R. Riebel (Emory University). Wiley-VCH, Weinheim, Germany. **2004**.
3. The Organic Chemistry of Enzyme-Catalyzed Reactions by R. B. Silverman, Academic Press, New York, **2000**.
4. Asymmetric Organocatalysis – From Biomimetic Concepts to Applications in Asymmetric Synthesis By A. Berkessel and H. Groger. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, **2005**.
5. Enantioselective Organocatalysis: Reactions and Experimental Procedures Edited by Peter I. Dalko Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, **2007**.
6. Organocatalysis Reetz, M.T.; List, B.; Jaroch, S.; Weinmann, H. (Eds.) Series: Ernst Schering Foundation Symposium Proceedings 2007-2 , Publisher: Springer-Verlag, Berlin Heidelberg, **2008**.
7. Advanced Inorganic Chemistry F.A Cotton 6th addition chapter 21 and 22, p. 1167-1294
8. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th edition a John Wiley & Sons, Inc., Publication, **2005**.
9. C. Elschenbroich and A. Salzer, Organometallics: A concise Introduction, 2nd Ed., VCH, **1992**.

**BIOPHYSICAL CHEMISTRY
CYL902****Credits: 3-0-0****Mid Semester Examination: 20% weightage****End Semester Examination: 80% weightage****Instructions for the Paper Setters:**

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

Section A**(11 Hrs)****1. Forces & Interactions in Aqueous Solutions:**

The denaturation of proteins; e.g denaturation of trypsin, the probabilities of the native & denatured states of a protein, thermal melting of proteins.

Hydrogen bonds; Equilibrium constants for intra- and intermolecular peptide hydrogen bonds. Non-polar & Electrostatic interactions; hydrophobic interactions in micelles & proteins, estimation of the strength of non-polar interactions. The basis of non-polar interactions; hydrophobic interactions, cold denaturation, dispersion interactions, Electrostatic interaction.

Section B**(11 Hrs)**

2. Protein-protein and protein-ligand interactions; physical and chemical method for study, kinetics of protein folding-unfolding, equilibrium effect of temperature and solvent conditions on the thermodynamics of protein folding-unfolding equilibrium.

Section C**(11 Hrs)****3. Techniques for the Study of Biological Structure and Function:**

Spectroscopic techniques; magnetic resonance methods (epr, nmr), other optical techniques; Rotatory behaviour of macromolecules, circular dichroism (CD) and optical rotatory dispersion (ORD).

Thermal Techniques; Differential Scanning Calorimetry, Isothermal Titration Calorimetry.

Section D**(12 Hrs)****4. Mechanism of Enzyme Catalysis:**

Factors responsible for catalytic efficiency of enzymes and nature of enzyme active site; Kinetics of enzyme catalyzed reactions, Theories of enzyme catalysis: rate enhancements, transition state stabilization, transition state analogues, catalytic antibodies, substrate specificity and induced fit, testing theories of catalysis, Example of enzyme mechanisms: lysozyme. allosteric enzymes; and kinetics of enzyme inhibitors;

Enzyme catalysis in solution-kinetics of thermodynamic analysis, effects of organic solvents on enzyme catalysis and structural consequences.

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Books Recommended:

1. Biochemistry, R.H. Abales, P.A. Frey and W.P. Jencks.
2. Biophysical Chemistry, (vol. I & II) by Cantor and Schimmel.
3. Principles of Biophysical Chemistry, van Holde.
4. Biochemistry, Voet and Voet, John Wiley.
5. Proteins: Structure and Molecular Properties, T.E. Creighton.
6. Biological Thermodynamics, D.T. Haynie.

Pre Ph.D. Course in Chemistry (CBE & GS)

SUPRAMOLECULAR CHEMISTRY
CYL903

Credits: 3-0-0

Mid Semester Examination: 20% weightage

End Semester Examination: 80% weightage

Instructions for the Paper Setters:

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

Section-A

1. Introduction

(11 Hrs)

What is supramolecular chemistry? Selectivity, The 'Lock and Key' Principle and Induced Fit Model, Complementarity, Cooperativity and the Chelate Effect Preorganisation, Binding Constants, Kinetic and Thermodynamic Selectivity, Solvation Effects, Supramolecular interactions, Ionic and dipolar interactions, Hydrogen bonding, π -interactions, Van der Waal's interactions, Close packing in the solid state, Hydrophobic effects, Supramolecular design.

Section-B

2. Solution Host-guest Chemistry-I

(12 Hrs)

Introduction: guests in solution, Macrocyclic versus acyclic hosts, High Dilution Synthesis, Template synthesis, synthesis of 18-crown-6, 2.2.2.cryptand, calix[4]arene, thiacalix[4]arene, spherands, Cation binding, Crown Ethers, Lariat Ethers, Cryptands, Spherands, Hemispherands, Cryptaspherands, Heterocrowns and Heterocryptands, Schiff's Bases, Calixarenes, Anion binding, Charged Receptors, Electrostatic Interactions, Electrostatic and Hydrogen Bonding Interactions, Neutral Receptors, Hydrogen-Bonding Interactions, Ditopic receptors, Neutral-molecule binding,

Section-C

3. Solution Host-guest Chemistry-II

(4 Hrs)

Supramolecular catalysis and enzyme mimics, Calix[4]arenes and Cyclodextrins as catalysts. Use of spectral techniques like NMR, UV and fluorescence in analytical sensing

4. Supramolecular Polymers, Gels and Fibres

(7 Hrs)

Introduction, Dendrimers, Covalent Polymers with Supramolecular Properties, Self-Assembled Supramolecular Polymers, Polycatenanes and Polyrotaxanes, Supramolecular Gels, Polymeric Liquid Crystals.

Section-D

5. Molecular Devices

(11 Hrs)

Introduction, Supramolecular Photochemistry, Information and Signals: Semiochemistry and Sensing, Molecule-Based Electronics, Photochemical devices, Molecular Wires and Rectifiers, Molecular Switches, Molecular Muscle, Towards Addressable Nanodevices, Nonlinear Optical Materials.

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Books:

1. Supramolecular Chemistry, 2nd Edition, March 2009 by Jonathan W. Steed, Jerry L. Atwood
2. Core Concepts in Supramolecular Chemistry and Nanochemistry, by J. W. Steed, D. R. Turner and K. J. Wallace, Wiley, 2007,
3. Chem. Rev., **2010**, 110 (4), pp 1960–2004.

CYL904: Research Methodology**L T P**
4 0 0**Mid Semester Examination: 20% weightage**
End Semester Examination: 80% weightage**Instructions for the Paper Setters:**

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Section A

Research Aptitude: Meaning of Research, Objectives of Research, Motivation in Research, Types of Research, Research Approaches, Research Methods versus Methodology, Research and Scientific Method, Importance of Knowing How Research is done.

Section B

Research Process: Reviewing the literature, Formulation of research problem, Nature and type of variables, Hypothesis - meaning, types, development of hypothesis and its testing, Meaning & Functions of Research Design

Data Analysis: Sources, acquisition and interpretation of data, Quantitative and qualitative data, Graphical representation and mapping of data, Sensitivity Analysis with Data Tables, Optimization with EXCEL Solver, Summarizing Data with Histograms and Descriptive Statistics, Pivot Tables, Summarizing Data with database statistical functions, using correlation, Multiple Regression, Using Sampling to Analyze Data

Section C

Significance of Report Writing: Different Steps in writing Report, Layout of the Research Report, Types of Reports, Mechanics of Writing a Research Report, Art of scientific writing- Steps to better writing, flow method, organization of material and style, Drawing figures, graphs, tables, footnotes, references etc. in a research paper

Section D

Use of internet in research work : Use of internet networks in research activities in searching material, paper downloading, submission of papers, relevant websites for journals and related research work. Introduction to Patent laws etc., process of patenting a research finding, Copy right, Cyber laws.

References:

1. *Research Methodology Methods and Techniques*, Kothari, C. R., Wiley Eastern Ltd.
2. *Microsoft Excel Data Analysis and Business Modeling*, Wayne L. Winston, Microsoft Press, ISBN: 0735619018
3. *Research Methodology: a step-by-step guide for beginners*, Kumar, Pearson Education.
4. *Practical Research Methods*, Dawson, C., UBSPD Pvt. Ltd.
5. *Research Methodology*, Sharma, N. K., KSK Publishers, New Delhi.

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References:

1. Bailey, N.T.J. (1995). *Statistical Methods in Biology*. Cambridge University Press, Cambridge.
2. Kothari, C.R. (2004). *Research Methodology: Methods and Techniques*, New Age International Publishers, New Delhi.

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GOOD LABORATORY PRACTICES
ESL964

Credits 3-0-0

(45 hrs.)

Mid Semester Examination: 20% weightage

End Semester Examination: 80% weightage

Instructions for the Paper Setters:

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

Section-A

(11 hrs.)

1. **Introduction to chemical analysis:** Nature of analytical chemistry, general directions of chemical analysis: Cleanliness in the laboratory, Recording and planning data. Data quality: Bias, Precision, Uncertainty, Method detection limit, Checking correctness of analysis, Expression of results, Significant figures, Collection and preservation of sample.

Section-B

(11hrs.)

2. **Laboratory hazards:** Chemical, Fire, Careless habits, Handling of compressed gases, Stockroom safety rules, Laboratory safety rules. Quality assurance of chemical measurements: Quality assurance, quality control, Quality assessment, Sampling, Sampling custody, Sample preparation, Analytical methodology with case studies, Calibrations, Detection limits, Statistics in chemical analysis, Quality control charts.

Section-C

(7hrs.)

3. **Laboratory apparatus and glassware:** Labware materials, soft vs. heat resistant glassware, plastic, porcelain, platinum, nickel labware. Volumetric flask, pipette, burette, cleaning of volumetric glassware. Types of balances: Analytical balances, Desiccators.

(4hrs.)

4. **Chemical reagents and standards:** Grade and purity of chemicals, Proper storage of chemicals and standards, Laboratory pure water, Preparation of reagent grade water, Reagent water quality.

Section-D

(3hrs.)

5. **Reagents and solutions.** Stock standardization solutions, Preparation and standardization of common standard solutions,

(6hrs.)

6. **Filtration:** Gravity, Vacuum, Centrifugation, Distillation: Simple, Fractional, Vacuum, Refluxing, Ion exchange, Drying and washing sample, Liquid-liquid extraction by separating funnel, Soxhlet extraction.

(3hrs.)

7. Software's for stock room management, Role of computers in Laboratory occupational health and safety, Waste minimization and disposal.

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References:

1. Csuros, M., Environmental Sampling and Analysis, Lewis Publications.
2. Standard methods for the examination of water and wastewater, American Public Health Association, 19th ed., Washington D.C.

Note: For courses LSL901 and ESL964 students will attend classes in Department of Botanical and Environment Sciences.

**EXPERIMENTAL TECHNIQUES
PHL902****LTP
3-0-0****Mid Semester Examination: 20% weightage
End Semester Examination: 80% weightage****Instructions for the Paper Setters:**

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Section-A

Physical basis, theory, instrumentation and applications of X-Ray Fluorescence Spectroscopy; LASER fluorimetry; Gamma-Gamma method; Neutron activation analysis and Neutron-Neutron method.

Section B

Gamma ray spectrometric technique for uranium, thorium and potassium analysis. Alpha particle track etch detector.

Section-C

Physical vapour deposition techniques : Thermal evaporation, Electron Beam Gun, Pulse Laser, Sputtering, Synthesis of bulk and nano structured materials using sol-gel technique.

Section-D

Spectroscopic Characterisation techniques; Infra Red (IR), UV-Visible, Raman and Photoluminescence spectroscopy. Atomic force microscopy, Transmission electron microscopy, Scanning electron microscopy, Energy dispersive X-Ray analysis, X-Ray diffraction.

References:

1. Radiation Detection and Measurements: Glenn F. Knoll.
2. Principles and Methods of Nuclear Geophysics: U.L.S. Bhima Shankran.
3. X-ray Fluorescence Spectroscopy: R. Jenkins-Wiley Interscience, New York, 1999.
4. Spectrometric identification of organic compounds: R.M. Silverstein
5. Methods of Surface Analysis : J.M. Walls- Cambridge University Press, 1989.
6. Modern techniques for surface science: D.P. Woodruff and T.A. Delchar- Cambridge University Press, 1994.
7. Thin Film Fundamentals: A. Goswami-New age International, 2007.
8. The Principles and Practice of Electron Microscopy: Ian. M. Watt- Cambridge University Press, 1997.

Disaster Management
ESL961

Credits 3-0-0

Mid Semester Examination: 20% weightage

End Semester Examination: 80% weightage

Instructions for the Paper Setters:

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

1. Introduction to disasters, common terminologies. Management acts, policies & institutions in India.
2. Earthquakes
Damage Prevention and Rehabilitation by
Retrofitting Dos and Don'ts While Constructing
Buildings Case study-Bhuj Earthquake 2001

SECTION-B

3. Floods
Standard Operating Procedure for Administration
Standard Operating Procedure for Individuals
Case study-Assam Floods 2004
4. Cyclones
Case study-Orissa Super Cyclone 1999
5. Droughts

SECTION-C

6. Landslides
7. Fire disasters-Forest Fires
Case study-Peerchu Lake – A Disaster in Being Kumbakonam School Fire Tragedy
8. Avalanches
9. Tsunami
Case study-Tsunami 2004

SECTION-D

9. Nuclear Disasters
Dos and Don'ts While Commercial Nuclear
Disaster
10. Chemical and industrial Disasters
Chemical and Industrial Disaster Mitigation
Case study-Bhopal Gas Tragedy 1984

Note: Related Case Studies can be included as per the topic.