DEPARTMENT OF CHEMISTRY
M.PHIL/PHD COURSEWORK SYLLABUS

COURSE STRUCTURE & CREDITS

Course No	**Name of Paper**	**L**	**T**	**P**	**Credits**	**Marks**
1st Semester						
CHE-RS-C101	Research methodology	3	1	0	4	100
CHE-RS-C102	Research Proposal Preparation	0	1	3	4	100
CHE-RS-Exxx	Elective	3	1	0	4	100
2nd & 3rd Semester						
CHE-RS-C201	M.Phil. Dissertation	0	0	12	12	
Total		6	3	15	24	

L: Lecture hrs/week, **P**: Practical hrs/week, **T**: Tutorials hrs/week,

ELECTIVES

CHE-RS-E101	Advanced Physical Chemistry
CHE-RS-E102	Advanced Topics in Organic Chemistry
CHE-RS-E103	Bio-Inorganic Chemistry
CHE-RS-E104	Computational Chemistry
CHE-RS-E105	Food Chemistry
CHE-RS-E106	Nanoscience
CHE-RS-E107	Soil Chemistry
CHE-RS-E108	Strategies in Organic Synthesis
CHE-RS-E109	Supramolecular Chemistry

SEMESTER I
CHE-RS-C101: Research Methodology

Unit I: Basic principles, health and safety, working with liquids

Basic laboratory procedures, Principles of solution chemistry, pH and buffer solutions. Principles of Green Chemistry and its practices.

Making and recording measurements, SI units and their use, Scientific method and design of experiments, Project works.

Using graphs, presenting data in tables, Hints for solving numerical problems, Descriptive statistics, choosing and using statistical tests, drawing chemical structures, chemometrics, error analysis – standard deviation, variance and various methods of error analysis

Unit II: The Internet and World Wide Web

Internet resources for chemistry, using spreadsheets, word processors, databases and other packages, finding and citing information.

General aspects of scientific writing, writing essays, writing articles, communications and reviews for journals, reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation examination.

Unit III: Meaning of research problems

Sources of research problems, criteria / characteristics of a good research problem, errors in selecting a research problem.

Format of research proposal, individual research proposal and institutional proposal. Format of the research report, style of writing the report, references and bibliography.

Unit IV: General safety and operational rules

Safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares, centrifuge safety, treated biomedical wastes. Emergency response, Chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency accident reporting.

Ethics and Human Interface: Essence, determinants and consequences of Ethics in human actions; dimensions of ethics; ethics in private and public relationships. Scientific and Professional ethics.

References

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., and Jones, A. 2002 Practical Skills in Chemistry, Pearson Education Ltd. [Prentice Hall]
2. OSU safety Manual 1.01.
3. Kothari, C. R. Research Methodology. Methods and Techniques
4. Singh, A. K. Tests, Measurements and Research Methods in Behavioural Sciences:

CHE-RS-C102: Research Proposal Preparation

Unit I: Presentation of scientific papers
Presentation of the recently well cited scientific research studies from journals of high impact factor. Topics of the presentation to be decided by students in consultation with teachers. Students should be presenting more than once in different areas.

Unit II & III: Research proposal
The students will write a detailed proposal of their research including a thorough review of literature on a topic of their choice and present the same in a seminar at least 10 days before the End-Sem examination.

Unit IV: Presentation on Instrumentation techniques
This unit seeks to update student's knowledge about the various instrumentation techniques relevant to his/her research work.

CHE-RS-E101: Advanced Physical Chemistry

Unit I: 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 II: Molecular collisions
Scattering as a probe of collision dynamics, Potential energy surface, Experimental techniques in reaction dynamics: molecular beam and chemiluminescence techniques, trajectory calculations, state to state kinetics, some case studies.

Unit III: Lasers: its properties and applications in reaction kinetics
Techniques for the study of fast and ultrafast reactions: Flow and stooped flow technique, relaxation technique, pump-probe technique , single photon counting and fluorescence up-conversion techniques, femtochemistry.

Unit IV: 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.

References

1. Prigogine, I. Introduction to Thermodynamics of Irreversible Processes.
2. Levine, R.D. and Bernstein, R.B. 1987 Chemical kinetics and dynamics Molecular Reaction Dynamics and Chemical Reactivity, Oxford
3. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part I: The Conformation of Biological Macromolecules.
4. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part II: Techniques for the Study of Biological Structure and Function
5. Cantor, C. R. Schimmel, P. R. Biophysical Chemistry: Part III: The Behavior of Biological Macrolmolecules
6. Somorjai, G.A. Li, Y. Introduction to Surface Chemistry and Catalysis

CHE-RS-E102: Advance Topics in Organic Chemistry

Unit I: Advanced Analytical Techniques

All advanced analytical techniques for structure determinations.

Unit II: Preparative techniques

Pyrolytic methods; chemical strategies, chemical vapour deposition; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructuress.Composition and purity of materials.

Conducting organics-Metals from molecules, charge transfer materials and conducting polymers. Organic superconductors. Fullerenes, Carbon nanotubes and graphene.Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphicbehaviour, optical properties of liquid crystals, display devices. Organic light emitting diodes.

Unit III: Synthetic Medicinal chemistry

Methods of combinatorial chemistry, solid phase synthesis, different types of polymer supports, linkers, strategies of library synthesis, characterization, diversity oriented synthesis, examples.

Unit IV: Stereoselective Synthesis of Enantiomerically Pure Drugs

Biocatalyzed reactions, glycosidation reaction, antisense oligonucleotides

References

1. Silverstein, R. M. and Webster, F. X. Introduction to Spectrometric identification of organic compounds, 6th Ed. John Wiley and Sons.
2. Macomber, R. S. A Complete Introduction to Modern NMR Spectroscopy.
3. Burger's Medicinal Chemistry and Drug Discovery. 6 Volume Set
4. Williams, D. A., Foye, W. O. Lemke, T. L. Foye's Principles of Medicinal Chemistry
5. Nadendla, R. R. Principles Of Organic Medicinal Chemistry
6. Wilson, C. O. Gisvold, O. Block, John, J. H., Beale, M.Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry

CHE-RS-E103: Bio-Inorganic Chemistry

Unit I: The storage of iron, zinc, copper, vanadium, chromium, molybdenum, cobalt, nickel, and manganese

Transport of Iron, Zinc, copper, vanadium, chromium, molybdenum, and cobalt. Iron Biomineralization

Unit II: Biological Redox Components

Energy Storage and Release, Coupling Electron Transfers and Substrate Activation. Electron-transfer rates: Self-Exchange and Cross Reactions, Marcus Theory, Cross reactions of blue copper proteins.

Long-range electron transfer in proteins. Modified Metalloproteins

Transport through membranes, Anion and cation carriers; Coupled transport processes; Electron coupled transport; Proton coupled transport; Light driven transport; Transport via transmembrane channels.

Unit III: Biological Oxygen Carriers

Haemoglobin, hemocyanin, and hemerythrin. Redox chemistry of free molecular dioxygen. Geometry and electronic structure of coordinated dioxygen. General aspects of chemistry of dioxygenwith iron, copper and cobalt. Other Ligands for Biological Oxygen Carriers: carbon monoxide, nitric oxide, Isocyanide and nitroso species

Iron-sulfur proteins and models. Multi-site redox enzymes: Hydrogenase and Nitrogenase. Biological nitrogen fixation. FeMo cofactor

Unit IV: Coordination, Intercalation and hydrogen bonding

Fundamental Reactions with Nucleic Acids: redox and hydrolytic chemistry. A case study: tris(phenanthroline) metal complexes. Binding Interactions with DNA. Techniques to Monitor Binding. Applications of different metal complexes that bind nucleic acids. Nature's use of metal/nucleic-acid interactions.

Metal deficiency and disease. Toxic effects of metals, Metals used in diagnosis and chemotherapy. A case study of *cis*-Platin.

References

1. Hughes, M. N. 1981, Inorganic Chemistry of Biological Processes, 2nd Ed.John-Wiley & Sons, New York

2. Kaim, W. and Schwederski, B. 1995 Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York

3. Lippard, S. J. and Berg, J. M. 1994 Principles of Bioinorganic Chemistry, University Science Books,

4. Bertini, I., Grey, H. B., Lippard, S. J. and Valentine, J. S. 1998 Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi

5. Mukherjee, G. N. and Das, A. Elements of Bioinorganic Chemistry

CHE-RS-E104: Computational Chemistry

Unit I: Monte Carlo, Molecular Dynamics simulations and its applications to understanding of physical and chemical transformations

Methods based on Hartree-Fock, Configuration Interaction, Deriving one and two electron properties, Semi-empirical methods, Coupled Cluster theory, Density functional theory, TDDFT. QM/MM methods

Unit II: Basic molecular biology

Basic principles of biochemistry, energy conversion, enzymatic catalysis, and active transport, enzyme models, drug design, computational modeling.

Unit III: Introduction to Classical Monte Carlo

Molecular Dynamics Simulation and Softwares - DLPOLY, GROMACS, TOWHEE, NAMD.Introduction to Quantum chemistry softwares – NwChem, Gaussian.Visualization softwares – VMD, Povray.

Unit IV: Computer programming languages

C++, FORTRAN. Python, Shell scripting. Writing Monte Carlo, Molecular Dynamics codes for chemistry problems. Parallel programming techniques like Open MP, MPI

References

1. Pople, J.A. and Beveridge, D.L. 1971 Approximate Molecular Orbital Theory, McGraw
2. Hill, New York
3. Parr, R.G. and Yang, W. 1989 Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford
4. Longman, A. L. 1996 Molecular Modelling, London.
5. Hunt, R. and Shelley 1998 Computers and Common Sense, Prentice Hall, New Delhi
6. Rajaraman, V 1990 Computer Programming in Fortran-90 Prentice Hall, New Delhi
7. Dickson, T. R. 1968 Computer and Chemistry: introduction to programming and numerical methods
8. Detar, D. F. Benjamin, W. A. Computer programs for chemistry 1968-1969 New York Vol. 1-3
9. Jensen, F. 1999 Introduction to Computational Chemistry, John Wiley, New York.
10. Cramer, D. Wiley, J. 2002 Computational Chemistry (Theories and Models), New York.
11. Frenkel, D. and Smit, B. Understanding Molecular Simulation: From Algorithms to Applications
12. Allen, M. P. and Tildsley, D. J. Computer Simulation of Liquids

CHE-RS-E105: Food Chemistry

Unit I: Review of Proteins, Lipids and Carbohydrates

Sources. Physical properties, Chemical properties

Vitamins and Minerals: Different types of vitamins and its sources, vitamins Stability and Degradation; Different kinds of minerals and its sources; Different Main elements, trace elements and some non essential elements; Minerals in Food Processing

Unit II: Food Additives
Importance of additives, food colors, bases, anti-oxidant, thickening agents, humectants in our everyday life.

Unit III: Food Contamination
Possibility of contamination of food with toxic compounds.
Classification of Toxic Compounds in Food; Food Safety and Regulations; Rules and Regulation Set for Food Contamination

Unit IV: Alcoholic Beverage
Composition, processing, and kinds of alcoholic beverage
Fermented food; determine the composition, processing.

References

1. Belitz H.D. and Grosch, W. 1999 Food Chemistry, 2nd edition, Springer
2. Adams, M.R. and Moss, M.O. 2000 Food Microbiology Royal Society of Chemistry; 2nd edition
3. Damodaran, S., Parkin, K. L. and Fennema, O. R. Fennema's Food Chemistry, Fourth Edition (Food Science and Technology).
4. Lawley, R. and Curtis, L. and Davis. J. Food Safety Hazard Guidebook
6. Adams, M. Ensuring Safe Food: From Production to Consumption
7. Aguilera, J.M.; Simpson R.; Welti-Chanes, J.; Bermudez Aguirre, D.; Barbosa-Canovas, G.(Editors) Food Engineering Interfaces (Food Engineering Series).
8. Molecular Biological and Immunological Techniques and Applications for Food Chemists by Bert Popping, Carmen Diaz-Amigo and Katrin Hoenicke.

CHE-RS-E106: Nanoscience

Unit I: Introduction
Surface to volume ratio, crystal structures, basic properties. Length scale: de Broglie wavelength, Bohr radius, excitons, confinement regimes, The Fermi Energy, Kubo Gap, the mean free path in metals, charging energy. Size and shape-dependent electrical, magnetic and optical properties of metal, metal oxide and semiconductor nanoparticles. Quantum size effect, Superparamagnetism, Surface Plasmon resonance.

Unit II: Synthetic approaches
Top down and bottom up. Colloidal growth. Chemical synthesis, functionalisation and basic characterisation of metal, metal oxide and semiconductor nanoparticles. Core-shell / multishell nanoparticles. Properties and synthesis of Carbon nanotubes, grapheme, fullerene. Recent advances in synthesis of new materials and their synthetic strategies. Characterization of nanomaterials.

Unit III: Polymer-nanoparticle composite
Electrochemistry of colloidal nanoparticles.Band gap engineering in semiconductor nanocrystals, Carbon based nanoparticles, self assembled nanostructures. Atom and molecule manipulation. Application of nanoparticles in drug delivery, biological imaging of cellular and subcellular structures, catalysis, sensor, tracer, cancer treatment, photovoltaics, single molecule detection and LED. Introduction to nanotoxicology.

Unit IV: Model problems for quantum wells, wires and dots
Density of states. Quantum mechanical review; wavefunction, Schrödinger equation, Bands; The Kronig-Penny Model, metals, semiconductor, insulators; Interband transition.

References

1. Kuno, M. Introductory Nanoscience, 2011, Taylor & Francis Group.
2. Rigach, A. L. (Editor), Semiconductor nanocrystal quantum dots: synthesis, assembly and applications
3. Klimov, V. I. Semiconductor and Metal Nanocrystals: Synthesis and Electronic and Optical Properties (Optical Science and Engineering)
4. Thanh, N.T. K. and Sayed, M. A. 2012 El Magnetic Nanoparticles: From Fabrication to Clinical Applications
5. Huck, W. T. and Huck, Wilhelm T. S. (Editor) Nanoscale Assembly: Chemical Techniques
6. Dresselhaus, M. S, Dresselhaus, G. and Avouris, P. Springer-Verlag. Carbon Nanotubes : Synthesis, Structure, Properties, and Applications
7. Acklin, B. and Lautens, E. Magnetic Nanoparticles: Properties, Synthesis and Application**s**
8. Taurozzi, J. S 2011 Nanoparticle-polymer composite membranes: Synthesis, characterization, and environmental applications.
9. Karn, B. Colvin, V. and Alivasatos, P. 2004 Nanotechnology and the Environment.
10. Zhou, B. Hermans, S., Somorjai, G. A. (Editors)Nanotechnology in Catalysis Volumes 1 and 2

CHE-RS-E107: Soil Chemistry

Unit I: Soil-definition
Chemical composition, method of separation of inorganic and organic components of soil.
Clay minerals: X-ray diffraction, Fourier synthesis. Arrangement of ions in a crystal lattice – correlation between ionic radii and coordination number.Different types of clay minerals, identification, their structures and structural formulas.Weathering: genesis of clay minerals, processes and products of weathering. Packing of coordinated units in a crystal lattice.Crystal structure of the silicates.

Unit II: Humic acid, Fulvic Acid
Their genesis. Structures – molecular weight of the organic components, determination of high molecular weights.Computer simulation of the structure of the organic components.

Surface charge, double layer theory.Adsorption/desorption: Langmuir adsorption isotherm. Derivation of the Langmuir equation for Ion-exchange Reactions in soils using statistical mechanics.Application and misapplication of the Langmuir equation to the soil adsorption phenomena.A general treatment and classification of the Solute Adsorption Isotherm.

Unit III: Cation exchange capacity

Causes of cation exchange capacity.Positions of exchangeable cations.Rate and environment of exchange reactions. Replaceability of exchangeable cations, Anion exchange
Soil redox potential - Some practical implications

Unit IV: Soil Fertility - An overview

A Quantity/Intensity approach to ion availability, Potassium Chemistry; Phosphorus Chemistry; Biogeochemistry of soil nitrogen; Biogeochemistry of soil sulfur; Evaluation of fertility status; Pollution problems

References

1. McBride, 1994 Environmental Chemistry of Soils, Oxford
2. Tan, Dekker, M. 1993 Principles of Soil Chemistry
3. Dixon and Weed, 1989 Minerals in Soil Environments, Soil Sci.
4. Sparks, 1989 Kinetics of Soil Chemical Processes, Academic Press
5. Wild and Longman, 1988 Russell's Soil Conditions and Plant Growth
5. Davis and Hayes Geochemical Processes at Mineral Surfaces, American Chemical Soc.,
6. Harter, Van Nostrand Reinhold, 1986 Adsorption Phenomena,
7. Sparks, 1986. Soil Physical Chemistry, CRC Press,
8. Bohn, McNeal, & O'Connor 1985 Soil Chemistry, 2nd Ed, Wiley Interscience.
9. Sposito, 1984. The Surface Chemistry of Soils, Oxford Press.
10. Lindsay, 1979 Chemical Equilibria in Soils, Wiley Interscience,
11. Alexander, 1977 Soil Microbiology, Wiley Interscience.

CHE-RS-E108: Strategies in Organic Synthesis

Unit I: Umpolung

Reaction by Organometallic Reagents, Sigmatropic Rearrangements, Pericyclic reactions, reactions of carbenes, Benzyne, Coupling reactions – Heck, Suzuki, and related, Wittig, Tebbes, Petasis, Grubbs, Peterson reactions, Simmon-smith reactions, radical reaction,
Hetero-atom alkylation or acylation, Nucleophilc substitution or addition by hereoatom nucleophiles, Mitsunobu reaction, pericyclic reactions, nitrenes.

Unit II: Reagents for Oxidation

Reduction, elimination, addition, organo silicon, organotin reagents, organo boron, organo-phosprus, organosulfur, organoselenium, Titanium, Fluorinating agents, Important starting materials and intermediates

Unit III: Methods of determining atropisomerism

Biphenyls, quasiracemates, dynamic stereochemistry, Axial chirality, planar chirality, helical chirality, determination of absolute configuration, Conformational analysis based on physical properties and chemical reactivity, shape of small and medium ring, Steroselectivity
Asymmetric synthesis using chiral pool, chiral auxiliaries, chiral reagents and chiral catalysts

Unit IV: Retrosynthetic strategies
Transform-Based Strategies, Structure-Goal Strategies, Topological Strategies, Stereochemical Strategies, Functional Group-Based Strategies. Choosing one path over other: Consideration of yield, availability of synthone, mildness of any reaction, Retrosynthesis and total synthesis of various natural products

References
1. Carey, F.A. and Sundberg, R.J. Advanced Organic Chemistry, Fourth Edition, Part A and B
2. Clayden, Greeves,Warren and Wothers, Organic Chemistry
3. March, J. 6th Edition, Advanced organic chemistry.
6. Carruthers, –W. Some modern methods of organic synthesis, Cambridge
7. Eliel, E. L. Stereochemistry of carbon compounds.
8. Fuhrhop, J.-H., Li, G., Corey, E. J. Organic Synthesis: Concepts and Methods.
9. Organic Synthesis: Concepts, Methods, Starting Materials, 2nd Edition, Jürgen-Hinrich Fuhrhop, Gustav Penzlin
10. Wyatt, P. Warren, S. Workbook for Organic Synthesis: The Disconnection Approach.

CHE-RS-E109: Supramolecular Chemistry

Unit I: Quantification of non-covalent forces and medium effects
Host design; Preorganization; Enthalpy and entropic contributions; Cooperativity and allosteric effects; Induced fit; Complexation selectivity.
Introduction, Proteins and Foldamers: Single Molecule Self-Assembly, Biochemical Self-Assembly, Self-Assembly in Synthetic Systems: Kinetic and Thermodynamic Considerations, Self-Assembling Coordination Compounds, Self-Assembly of Closed Complexes by Hydrogen Bonding, Catenanes and Rotaxanes, Helicates and Helical Assemblies, Molecular Knots

Unit II: Lariat ethers and podands
Crown ethers, cryptands, calyx[n]arenes, cucurbit[n]urils, spherands; Selectivity of cationcomplexation; Macrocyclic, macrobicyclic and template effects
Concepts in anion host design; Guanidinium-based receptors; Organometallic receptors; Neutral receptors; Hydride sponge; Anticrowns; Biological Anion receptors
Binding by cavitands, cyclodextrins, cucurbit[n]urils, dendrimers, molecular clefts and tweezers, cyclophane Hosts

Unit III: Catalysis by cation, anion and neutral receptors
Supramolecular metallocatalysis; Cocatalysis; Biomolecular and abiotic catalysis.
Biological Inspiration for Supramolecular Chemistry, Alkali Metal Cations in Biochemistry, Porphyrins and TetrapyrroleMacrocycles, Supramolecular Features of Plant Photosynthesis,

Uptake and Transport of Oxygen by Haemoglobin, Enzymes and Coenzymes, Neurotransmitters and Hormones, DNA.

Unit IV: Solid-State Host-Guest Compounds

Clathrate Hydrates, Urea and ThioureaClathrates, Other Channel Clathrates, Hydroquinone, Phenol, Dianin's Compound and the Hexahost Strategy, Tri-o-thymotide, Cyclotriveratrylene, Inclusion Compounds of the Calixarenes, Solid-Gas and Solid-Liquid Reactions in Molecular Crystals.

Introduction, Supramolecular Photochemistry, Information and Signals: Semiochemistry and Sensing, Molecule-Based Electronics, Molecular Analogues of Mechanical Machines, Nonlinear Optical Materials.

References

1. Steed, J. W. and Atwood, J. L. Supramolecular Chemistry John Wiley and Sons, Ltd.
2. Lehn, J.–M. Supramolecular Chemistry-Concepts and Perspectives, VCH.
3. Schnider. H.-J. and Yatsimirsky, A.K. Principles and Methods in Supramolecular Chemistry John Wiley and Sons, Ltd.
4. Bianchi, A., James, K. B. and Garcia-Espana, E. Supramolecular Chemistry of anions, Wiley-VCH.
5. Teikink, E. R. T. and Vittal, J. J. Frontiers in Crystal Engineering.
6. Steed, J. W. and Atwood, J. L. Encyclopedia of Supramolecular Chemistry.
7. Cragg, P. J. A Practical Guide to Supramolecular Chemistry.
8. Steed, J. W., Turner, D. R. and Wallace, K. J. Core Concepts in Supramolecular Chemistry and Nanochemistry