DEPARTMENT OF CHEMISTRY FACULTY OF SCIENCE



UNIVERSITY OF RAJSHAHI

Syllabus for The Degree of Master of Science (M. Sc.) in Chemistry

> Session: 2018–2019 Examination 2019 [General Group] Examination 2020 [Thesis Group]

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THE HISTORY OF DEPARTMENT

The word "chemistry" has been derived from the Greek word "chemeia", meaning, "the art of metal working". Obviously modern chemistry involves a great deal more than this. It has become an interdisciplinary science, and today no scientific work can escape chemistry. Chemistry plays vital roles in our lives, namely agricultural products, chemicals, fertilizers, medicines and drugs, plastics, alloys, electronic components to paper, wood products etc.

The Department of Chemistry started functioning as a small discipline in 1958 in the First Science Building under the leadership of Late Dr. Kazi Abdul Latif with a batch of 15 postgraduate (Master Previous) students. The teaching was started in December 1958. A three year B.Sc. Honours course was initiated in 1962. The Department was shifted to its present location in the Second Science Building in 1968. Since then it has grown and flourished into one of the biggest departments of Rajshahi University. This growth was made possible by the dynamic leadership of the departmental staffs and availability of the financial support from various heads. The major cause in the sustained and rapid growth is the vitality of the faculty whose research interest includes programs of the frontiers of physical, organic, inorganic, analytical, polymer, industrial, agro-environmental chemistry and nanochemistry. The department is committed to provide stimulating graduate and postgraduate educations at the highest level of attainment. All the major areas of research thrust being pursued in the department are of theoretical significance as well as of practical utility.

The present enrolment of students at the B.Sc. Honours (4 years) and M.Sc. (one year/ two years) levels is about 500 including 12 M.Phil. and 9 Ph.D. fellows. At present there are 37 members of teaching staff and 40 supporting laboratory and office staff catering the needs of the students and the research scholars.

Mission

The Department of Chemistry is offering M.Sc. degree with specialization in three major branches of physical, inorganic and organic chemistry. Each branch offers M.Sc. degree in either of the two groups on the choice of students: a thesis group or a non-thesis group. In the thesis group a student has to undertake an independent research work (of 8 credits) under the supervision of a faculty member whereas a non-thesis student shall take the practical course of the respective branch.

Vision

On completion of M.Sc. degree the Department of Chemistry is committed to produce a scientifically literate working force having deep understanding of chemical knowledge to satisfy the demands of employers, institutes (research and education) and industries. They will be able to design new materials and can solve the global problems facing in industrial, environmental, health and technological sectors. It is also expected that they will have enduring passion to learn more through engaging in creative research for higher degrees like M.Phil. and Ph.D.

M.Sc. Examination, 2019 [General Group] M.Sc. Examination, 2020 [Thesis Group]

PHYSICAL BRANCH

The Courses and distribution of marks are as follows:

Courses	Course Titles		<u>Units</u>	<u>Credits</u>	<u>Marks</u>
Chem 511F	Electroanalytical Chemistry		1.0	4	100
Chem 512F	Advanced Chemical Spectroscopy		1.0	4	100
Chem 513F	Pharmacokinetics		1.0	4	100
Chem 514F	Biophysical Chemistry		1.0	4	100
Chem 515F	Physical Chemistry of Polymers		1.0	4	100
Chem 516F	Nanomaterials and Nanochemistry		1.0	4	100
Chem 517F	Theoretical Chemistry		1.0	4	100
Chem 511VF	Viva-voce		1.0	4	100
Chem 511L*	Physical Chemistry Practical		2.0	8	200
	OR				
Chem 599**	Thesis / Dissertation on topics of		2.0	8	200
	Physical Chemistry				
		Total	9.0	36	900

Students shall have to choose **any six full unit theoretical courses from the first seven full unit theoretical courses** (Chem 511F– Chem 517F) subject to the approval of the branch.

* Laboratory courses include 30% (60) marks for continuous Lab. assessment.

** Thesis includes 25% marks (50 marks) for oral examination on thesis.

The M.Sc. Program in Chemistry for General Group shall extend over a period of one academic year and for Thesis Group shall be of two academic years. The final

examination on theory courses for both General and Thesis Groups shall be held together at the end of one academic year.

All theory courses include 80% final examination and 20% in-course. The **Final examination** of 80% of each 100 marks (1.0 unit, 4 credits) theory full course shall be of 4 (four) hours duration. In-course comprises of 15% tutorial or terminal and 5% class attendance. The class **teachers** of each course shall submit the average marks of in-courses in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last class held. The relevant **examination committee** shall prepare the result by adding the average marks of each in-course to the average marks obtained in the final examination of respective course, and send a copy of the average marks of each in-course to the controller of examinations.

The practical course includes 70% practical examination and 30% continuous Lab assessment. The practical examination of 70% of 200 marks (2.0 units, 8 credits) practical course shall be of 24 (twenty four) hours duration (4 days). The students are required to submit a report after each practical class to the class teacher(s) for evaluation. After evaluation the report shall be returned to the students. The class **teacher(s)** shall submit the average marks of all Lab evaluation in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last Lab class held. The examination committee shall send a copy of each of the consolidated **practical** and **Lab evaluation** marks to the **controller** of examinations.

Viva-voce examination (**Chem 511VF**) includes the assessment of the students through oral examination (of all the courses) by the **members** of the relevant examination committee. The **examination committee** shall send a copy of the marks to the **controller** of examinations.

N.B.: Students having less than 60% class attendance shall not be allowed to sit for the examination.

Course: Chem 511F Electroanalytical Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course illustrates the basic principles and applications of modern electroanalytical methods at the advanced level. It helps students to understand the basic principles of electrochemistry involved in various electroanalytical techniques. As a consequence, they will be able to apply the electroanalytical techniques for analytical applications.

- 1. **Kinetics of Electrode Processes (13 lectures).** Faradic and non-Faradic processes; mass transport-controlled reactions; electrode polarization and overpotential; classification of polarization phenomenon, the concept and theory of diffusion overpotential; diffusion-controlled reactions; principles and applications of polarography; basic factors in ion discharge; formulation of overall kinetic rate equation, concentration dependence of rate of a discharge step, net currents and exchange currents; heats of activation and frequency factors; activation controlled reactions; kinetics and mechanism of some simple electrode reactions, viz., hydrogen evolution at the cathode and oxygen evolution at the anode.
- 2. Electrode Reactions in Cyclic Voltammetry (12 lectures). Theory of cyclic voltammetry, interpretation of cyclic voltammogram; reversible, irreversible and quasi-reversible systems with single and multi-electron transfer; effects of pH, solvents and homogeneous chemical reactions on cyclic voltammetry; reaction mechanism: EC, E; adsorption processes; quantitative applications.
- 3. **Controlled Potential Techniques of Voltammetry (15 lectures).** Chronoamperometry, pulse voltammetry: normal pulse, differential pulse, squarewave, and stair case voltammetry. Stripping voltammetry: stripping analysis; anodic, potentiometric and adsorptive voltammetry and potentiometry, cathodic stripping voltammetry and its applications. Flow analysis: principles, cell design, mass transport and current response, detection modes.
- 4. Electrodes of Electrochemical Cells (10 lectures). Solvent and supporting electrolytes, oxygen removal, instrumentation working electrodes viz, mercury electrodes; solid electrodes, rotating disk electrodes, carbon electrodes: glassy-

carbon, carbon-paste and carbon-fiber electrodes, metal electrodes, chemically modified electrodes: self-assembled monolayers, sol-gel encapsulation of reactive species, electrocatalytic modified electrode, pre-concentrating electrodes, pre-selective coatings, conducting polymers, microelectrodes: diffusion at microelectrodes, configurations of microelectrodes, composite electrodes.

- 5. **Potentiometry (10 lectures).** Principles of on line and in-vivo potentiometric measurements using ion selective electrodes, glass electrodes, pH electrodes, glass electrodes for other cations, liquid membrane electrodes, solid state electrodes and coated wire electrodes.
- 6. Electrode Modification and Electrochemical Sensors (10 lectures). Biosensors (enzyme-based electrodes), impractical and theoretical considerations, enzyme electrodes of analytical significance e.g. glucose sensors, ethanol and urea electrodes, toxin (enzyme inhibition) biosensors, tissue and bacteria electrodes. Affinity biosensors (immunosensors, DNA hybridization biosensors, receptor based sensors), gas sensors: carbon dioxide sensors, oxygen electrodes, solid-state devices: microfabrication of solid state sensor assemblies, microfabrication techniques, sensor arrays.
- 7. Applied Electrochemistry (10 lectures). Corrosion and passivation of metals, corrosion testing, corrosion industries, theories of corrosion and methods of combating corrosion; electrochemical energy conversion devices, primary and secondary batteries, fuel cells, electroplating of metals, viz., Cu, Ni, and Cr; factors governing the nature of deposits; ornamental and porous deposits

- 1. Joseph Wang: Analytical Electrochemistry
- 2. A.J. Bard.: Electrochemical Methods: Fundamentals and Applications
- 3 Peter T. Kissenger and William R. Heineman: Laboratory Techniques in Electroanalytical Chemistry
- 4. Royce W. Murray: Molecular Design of Electrode Surfaces
- 5. A.E.G. Cass: Biosensors
- 6. J.J. Lingane: Electroanalytical Chemistry
- 7. Fred C. Anson: Electroanalytical Chemistry
- 8. Mars G. Fontans and Greene: Corrosion Engineering
- 9. J.O'M. Bockris and A.K.N. Reddy: Introduction to Electrochemistry
- 10. B.E. Conway: Electrode Processes
- 11. K.J. Vetter: Electrochemical Kinetics

Course: Chem 512F Advanced Chemical Spectroscopy Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course emphasizes on the basic principles and applications of atomic and molecular spectroscopy. It helps students to understand the common spectroscopic techniques used in structure determination and analytical purposes. Students will be able to apply the knowledge for quantitative analysis of samples and to identify unknown molecules from a given set of characteristic spectra. Students will use spectroscopic data to make meaningful observations about the chemical properties of compounds.

- Atomic Spectrometry (22 lectures). Theory of Atomic Spectroscopy: basic 1. principles, fundamentals of absorption and emission: absorption; line broadening; self-absorption; ionization; dissociation; radiation sources and atom reservoirs. Atomic Absorption Spectrometry (AAS): instrumentation: radiation sources; atomizers; optical set-up and components of atomic absorption instruments, spectral interference: origin of spectral interference; methods for correcting for spectral interference, chemical interferences: formation of compounds of low volatility; influence on dissociation equilibria; ionization in flames, data treatment: quantitative analysis, hyphenated techniques: gas chromatographyatomic absorption spectrometry; liquid chromatography-atomic absorption spectrometry. Atomic Emission Spectrometry (AES): instrumentation: atomization devices; optical set-up and detection; instrumentation for solid sample, matrix effects and interference: spectral interferences; matrix effects and chemical interferences, quantitative and qualitative analysis, advantages and limitations: absolute and relative sensitivity; hyphenated techniques.
- 2. Raman Spectroscopy (15 lectures). Classical and quantum theory; rotational Raman spectrum; instrumentation; effect of nuclear spin; molecules without a centre of symmetry; vibrational Raman spectra; mutual exclusion principles; polarization of Raman lines. Group theoretical analysis of vibrational spectra; vibrational analysis of single crystals; determination of structure by the application of Raman and infrared selection rules; vibrational-rotational Raman spectra; hyper Raman effect.

- **3.** Electron Spin/Paramagnetic Resonance (ESR/EPR) Spectroscopy (13 lectures). Introduction; principles; instrumentation; spectrum; hyperfine structure; radicals; anions of aromatic hydrocarbons; relation between hyperline-splitting and unpaired electron density; interpretation of ESR spectra; ESR spectra of transition metal complexes as single crystals; applications.
- **4.** Fluorescence Spectroscopy (12 lectures). Principle, instrumentation, transition probabilities and life time, quantum yield, fluorescence intensity and polarization, fluorophores and fluorescence probes, fluorescence parameters, molecular dynamics study and other applications.
- 5. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) (12 lectures). Optical activity and circularly polarized light; parameters for optical activity; measurement of ORD and CD; physical basis of optical activity; optically active chromophores; the use of CD to determine secondary structures.
- 6. Mössbauer Spectroscopy (6 lectures). Principle, factors affecting resonance of γ -ray absorption: nuclear recoil energy; Doppler effect; Mössbauer's contributions for resonance absorption, Mossbauer spectrum, instrumentation and sampling, hyperfine interactions: isomer or chemical shift; quadruple splitting; nuclear Zeeman or magnetic field effect, applications: nature of chemical bonding; molecular structure and studies on biological systems.

- 1. G. Gaunglitz and T. Vo-Dinh: Handbook of Spectroscopy
- 2. D.A. Skoog: Principles of Instrumental Analysis
- 3. B.P. Straughan and S. Walker : Spectroscopy
- 4. C.N. Banwell: Fundamentals of Molecular Spectroscopy
- 5. P.S. Sindhu: Molecular Spectroscopy
- 6. I.D. Campbell and R.A. Dwek : Biological Spectroscopy
- 7. D. Freifelder: Physical Biochemistry
- 8. D.C. Harris: Quantitative Chemical Analysis
- 9. D.A. Skoog, D.M. West and F.G. Holler: Fundamentals of Analytical Chemistry

Course: Chem 513F Pharmacokinetics Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course illustrates the basic concepts of pharmacokinetics including absorption, distribution, metabolism and excretion of a drug and the models used in pharmacokinetic study. The students will learn the physicochemical and physiological factors that influence the absorption of drugs, their distribution within the body, and their routes and mechanisms of elimination. Students will be able to apply the knowledge for new drug development, to study novel drug delivery system and to design dosage form.

- 1. **Introduction to Pharmacokinetics (10 lectures).** Processes in pharmacokinetics, plasma concentration of drugs, plasma level-time curve, measurement of drug concentrations, sampling of biologic specimens, significance of measuring plasma drug concentrations, pharmacokinetic models: compartment models, physiologic pharmacokinetic model (flow model).
- 2. Compartmental Models in Pharmacokinetics (15 lectures). One compartment model: Intravenous route of administration of drug, elimination rate constant, apparent volume of distribution, calculation of volume of distribution, significance of the apparent volume of distribution, calculation of k from urinary excretion data. Multicompartment models: two-compartment open model, method of residuals, apparent volumes of distribution, significance of the volumes of distribution, significance of the tissue compartment, elimination rate constant, three-compartment open model, determination of compartment models.
- 3. **Drug Absorption (20 lectures).** Physiologic factors: structure and properties of membranes, mechanism of drug absorption, factors affecting passive drug absorption, pH-partition theory of drug absorption, root of drug administration, rate limiting steps in drug adsorption, the effect of the dosage form (solution, suspension, capsule, tablet) on gastrointestinal absorption. Physicochemical factors: dissolution rate, dissolution process, Noyes-Whitney equation and drug dissolution, factors affecting the dissolution rate, dissolution methods, in vitro-in vivo correlation of dissolution.

- 4. **Drug Distribution and Protein Binding (13 lectures).** Physiological factors, diffusion and hydrostatic pressure, tissue perfusion and initial drug distribution, drug distribution and pharmacodynamics, effect of protein binding on the apparent volume of distribution, protein binding of drugs, kinetics of protein binding, determination of constant, relationship between protein concentration and drug concentration in protein-drug binding.
- 5. Pharmacokinetics of Drug Adsorption (10 lectures). Zero-order absorption model, first order absorption model, determination of absorption rate constants from oral absorption data: method of residuals, Wagner-Nelson method. Determination of k_a from two compartment oral absorption data, significance of absorption rate constant.
- 6. Non-linear Pharmacokinetics (12 lectures). Introduction, drug elimination by capacity-limited pharmacokinetics: one compartment model (IV bolus injection), estimation of Michaelis-Menten parameters (V_{max} and K_m), determination of clearance, time dependent pharmacokinetics.

Recommended Books:

- 1. Shargel, Susanna Wu-Pong and Andrew B.C. Yu: Applied Biopharmaceutics and Pharmacokinetics
- 2. Sara Rosenbaum: Basic Pharmacokinetics and pharmacodynamics
- 3. Sunil S Jambhekar and Philip J Breen: Basic pharmacokinetic
- 4. Martin, P. Bustamante and A.H.C. Chun: Physical Pharmacy

Course: Chem 514F Biophysical Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course is designed to introduce students to structure and functions of biomolecules. After successful completion of the course, the participant should have the ability to account for the structure and activities of biomolecules like peptides, proteins, carbohydrates and their interactions with the other components in the biofluids. The achieved knowledge will help the students in developing career in pharmaceutical industries, and to pursue higher studies in biochemical and biomedical science areas.

- 1. Noncovalent Bonding and pH Buffering (10 lectures). Water the biological solvent, stabilizing and organizing forces of nature, acid base equilibria, principle of pH buffering, buffering of blood, laboratory use of buffers, ionic strength.
- 2. Biomolecules (10 lectures). Building block molecules of biomolecules, amino acid structures, polypeptides, ionic properties of amino acids and polypeptides, nucleotides and nucleic acids, base composition and base sequence of nucleic acids, simple idea about carbohydrates and lipids.
- **3. Proteins (10 lectures).** Classifications, primary, secondary, tertiary and quarternary structure of globular proteins, salting in and salting out of proteins, chemistry of ion exchange and chromatographic technique in isolation/purification of protein, characterization of proteins, molecular weight determination of proteins by PAGE and get filtration techniques.
- 4. Enzymes (15 lectures). Nomenclature, cofactor, principle of catalysis, enzyme catalyzed reactions having one substrate, M-M equation, K_m and V_m values determination, pH and temperature effects on catalysis, competitive, non-competitive and uncompetitive inhibition of catalysis, transport of oxygen and CO₂ (the role of hemoglobin).
- **5. Bioenergetics (20 lectures).** ATP and its role in bioenergetics, control points in metabolic pathways, carbohydrate metabolism, the energetic of the citric acid cycle.
- 6. Specificity and Modifications of Proteins/Enzymes (5 lectures). Trypsin, chymotrypsin, elastase, carboxypeptidase, aminopeptidase, cyanogen bromide cleavage, SH, -S-S-, -NH₂, -SCH₃ group modification.
- 7. Biological Membranes (10 lectures). Constituents and structure, the fluid mosaic model, factors affecting the physical properties of membranes, the theory and thermodynamic of biological transport, energy coupling mechanisms in biological transport, molecular mechanism of biological transport.

- 1. A. W. Lehninger: Principles of Biochemistry
- 2. R.C. Bohinski: Modern Concepts of Biochemistry
- 3. G. Zubay: Biochemistry
- 4. D. Freifelder: Physical Biochemistry
- 5. R.K. Scopes: Protein Purification
- 6. C.N. Price and R.A. Dwek: Principles and Problems in Physical Chemistry for Biochemists
- 7. W.H. Elliott and D.C. Elliott: Biochemistry and Molecular Biology

Course: Chem 515F Physical Chemistry of Polymers Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course illustrates the physical properties of polymers. The student will learn the structure and properties of polymers in solution and in bulk state. They may be able to utilize the acquired knowledge to the field of polymer science and technology.

- 1. Basic Concepts of Polymers (25 lectures). The macromolecular concept; some basic terms and definitions: monomer, oligomer and polymer; repeating unit; end groups; degree of polymerization; representation of polymer structures, polymer nomenclature; polymer molecular weights and distributions; natural and synthetic polymers; polymerization and functionality principle; condensation and addition polymerizations; kinetics of polymerization; linear, branched and cross-linked (network) polymers. Isomerism in polymers: positional, stereo and geometrical isomerism. Copolymerization: random, block and graft copolymers and their technical significance.
- 2. Statistical Properties of Polymer Chains (15 lectures). Conformation of polymers; the ideal chain, fundamental properties of Gaussian chain, effect of internal rotation and stiff chains, excluded volume effect; Sealing laws and the temperature blob model; coil-globule transition and coil-helix transition of polymer chains, hydration of polymer chains.
- **3. Polymer Solutions (5 lectures):** Thermodynamics of phase equilibria; characteristic properties of polymer solutions; lattice theory of polymer solutions; Scaling laws of polymer solutions.
- Bulk Polymer State (10 lectures): Crystallization and melting of polymers; 4. thermal transition in polymers; crystallization: rate of crystallization, the Avrami equation, thermodynamics of polymer crystalligation, equilibrium melting temperature, primary nucleation, homogeneously and heterogeneous nucleation, nucleation, Laurigen-Hoffman secondary theory, crystal growth rate. crystallization regimes. kinetics of primary crystallization, secondary crystallization. The crystalline melting temperature: factors influencing melting, effects of chemical structure, intermolecular interactions, entropy and chain flexibility, solvent, structural defeats and molecular weights.
- 5. Glass Transition (T_g) of Polymers (5 lectures). Glassy solids and glass transition; free volume, viscosity and the glass transition; thermodynamic and

kinetic aspects of the T_g ; effect of molecular weights, chemical structure, crosslinking, crystallization and diluents; T_g of random copolymers and blends.

Recommended Books:

- 1. Alfred Rudin: The elements of Polymer Science and Engineering
- 2. P.C. Painter and M.M. Coleman: Essentials of Polymer Science and Engineering
- 3. Fumihiko Tanaka: Polymer Physics, Application to molecular Association and Thermorevesible Gentian
- 4. Michael Rubinstein and Ralph H. Colby: Principles of Polymer Physics
- 5. P.J. Flory: Principles of Polymer Chemistry

Course: Chem 516F Nanomaterials and Nanochemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course focuses on synthesis, characterization, common properties and applications of nanoparticles. Students will be familiar with the basic concept of nanochemistry and size dependent properties of nanoparticles, principles and characterization of nanoparticles. They may be able to apply the knowledge to the field of nanotechnology including biomedicine.

- Basic Concept and Nanoscale Phenomena (15 lectures). Concepts of nanoscale, nanoscience, nanotechnology and nanochemistry. Classification of nanomaterials. Size dependent properties: surface area, surface free energy, lattice parameters, phase transition, melting point, specific heat, quantum mechanics of nanomaterials – band structure; band gap; band splitting; electron density of states; optical properties – surface plasmon resonance; quantum size effects; electrical properties and superconductivity; magnetic properties and spintronics; mechanical properties – elasticity; hardness; ductility; superplasticity, chemical reactivity and catalytic activity.
- 2. Nanomaterial Characterization (15 lectures). Structural characterization: Xray diffraction (XRD), small angle X-ray scattering (SAXS), electron microscopy- interaction between electron beams and solids; transmission electron microscope (TEM); scanning electron microscope (SEM); scanning probe

microscope (SPM); gas adsorption. Surface analysis methods: auger electron spectroscope (AES), X-ray photoelectron spectroscope (XPS), secondary ion mass spectroscope (SIMS). Chemical characterization: optical spectroscopy, electron spectroscopy, ionic spectrometry, surface-enhanced spectroscopy: surface-enhanced vibrational spectroscopy; Surface-enhanced Raman scattering (SERS); surface-enhanced fluorescence spectroscopy.

- 3. **Top-down Approaches of Synthesis (15 lectures).** Thin-film deposition: homogeneous and heterogeneous film growth mechanisms, deposition methods–thermal deposition, molecular beam epitaxy, physical vapor deposition (PVD), chemical vapor deposition (CVD). Nanolithography: parallel replication, serial writing, electron beam lithography (EBL), nanoimprint lithography (NIL) NIL process; 3D patterning; air cushion press; sequential embossing/imprinting lithography (SEIL), AFM lithography– scratching and nanoindentation; nanografting, polymer pen lithography, templated self-assembly of block copolymers, focused ion beam (FIB) lithography, nanosphere lithography.
- 4. **Bottom-up Approaches of Synthesis (15 lectures).** Synthesis of nanoparticles: coprecipitation, sol-gel process, microemulsions, hydrothermal/solvothermal methods, templated synthesis, NPs of organic semiconductors. Self-assembly of nanoparticles: hydrogen bonding-based assembly, electrostatic assembly; shape-selective assembly; hydrophobic assembly, template-assisted assembly, collective properties of self-assembled.
- 5. Special Nanomaterials (10 lectures). Carbon fullerenes, fullerene-derived crystals, carbon nanotubes, graphen, silicon nanomaterials, micro and mesoporous materials ordered and random mesoporous structures; crystalline microporous materials (zeolites), core-shell structures metal-oxide structures; metal-polymer structures; oxide-polymer structures, organic-inorganic hybrids class I hybrids, class II hybrids: intercalation compounds, nanocomposites and nanograined materials.
- 6. **Applications of Nanomaterials (10 lectures).** Molecular electronics and nanoelectronics, nanobots, biomedical applications of nanoparticles, catalysis by nanoparticles, band gap engineered quantum devices quantum well and quantum dot devices, nanomechanics, carbon nanotube emitters, photoelectrochemical cells, photonic crystals and plasmon waveguides.

Recommended Books:

1. C. Brechignac, P. Houdy and M. Lahmani: Nanomaterials and Nanochemistry

- 2. Zhen Guo and Li Tan: Fundamentals and Applications of Nanomaterials
- 3. Guozhong Cao: Nanostructures and Nanomaterials Synthesis, Properties and Applications

Course: Chem 517F Theoretical Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO):

This course focuses on structure of molecules and quantum statistics. Upon completion of the course, students will be able to explain microscopic behaviors of substances. They will be able to design novel compounds and predict their properties.

- 1. Quantum Theory of the Chemical Bond Diatomic Molecules (25 lectures). Born-Oppenheimer approximation; nuclear motion in diatomic molecules; the hydrogen molecule ion (H_2^+) ; approximate treatments of H_2^+ ground electronic state; molecular orbitals for H_2^+ excited states; molecular orbital (MO) configurations of homonuclear diatomic molecules; electronic terms for diatomic molecules; the hydrogen molecule (H₂); valence-bond (VB) treatment of H₂; comparison of MO and VB theories; MO and VB wavefunctions for homonuclear diatomic molecules; excited states of H₂; electron probability density; dipole moments; the Hartree-Fock method for molecules; self-consistent-field (SCF) wavefunctions for diatomic molecules; MO and VB treatments of heteronuclear diatomic molecules; the valence electron approximation; configuration interaction (CI) wavefunctions.
- 2. Quantum Theory of the Chemical Bond Polyatomic Molecules (20 lectures). *Ab inito*, density-functional, semiempirical and molecular-mechanics methods; electronic terms of polyatomic molecules; the SCF MO treatment of polyatomic molecules; basis functions; the SCF MO treatment of H₂O; population analysis; the molecular electrostatic potential and atomic charges; localized MOs; the SCF MO treatment of methane, ethane, and ethylene; molecular geometry.
- 3. **\pi-Electron Theory of Organic Molecules (10 lectures).** Hückel MO theory; the use of symmetry for determining Hückel orbitals; cyclic conjugated polyolefins and Hückel's 4n + 2 rule; aromaticity and antiaromaticity; non-classical structures; heteroatomic molecules; the free electron model of π -electron molecules.
- 4. **Statistical Mechanics and Quantum Statistics (25 lectures).** Phase space and the Liouville's theorem; equipartition of energy. Quantum statistics: Boltzmann statistics, Fermi-Dirac and Bose-Einstein statistics, comparison of the three statistics; quantum statistics of weakly degenerate and strongly degenerate ideal

Fermi-Dirac gases, an ideal gas of photons (blackbody radiation); the density matrix; the classical limit from quantum mechanical expression for Q. Statistical thermodynamics of crystalline solids: vibrational spectrum of a monatomic crystal, Einstein and Debye theories of the heat capacity of crystals, lattice dynamics, phonons, and point defects in crystals. Theories of liquids: the theory of significant structures and the Lennard-Jones Devonshire theory.

Recommended Books:

- 1. Ira N. Levine: Quantum Chemistry
- 2. J.N. Murrel, S.F.A. Kettle and J.M. Tedder: Valence Theory
- 3. P.W. Atkins: Molecular Quantum Mechanics
- 4. Donald A. McQuarrie: Quantum Chemistry
- 5. H. Eyring, J. Walter and G.E. Kimball: Quantum Chemistry
- 6. R. Anantharaman: Fundamentals of Quantum Mechanic
- 7. A.K. Chandra: Introductory Quantum Chemistry
- 8. Donald A. McQuarrie: Physical Chemistry: A Molecular Approach
- 9. S. Glasstone: Theoretical Chemistry
- 10. Donald A. McQuarrie: Statistical Thermodynamics
- 11. Gurdeep Raj: Advanced Physical Chemistry

Course: Chem 511L Physical Chemistry Practical Examination: 24 hours (4 days) Full Marks: 200 (2.0 unit, 8 credits) (i) Experiment: 140 Marks, (ii) Continuous Lab. assessment: 60 Marks

[N.B. In addition to the experiments listed below more experiments on physical chemistry may be done subject to the availability of the Lab. facilities.]

Intended Learning Outcomes (ILO)

This course concerns with some experiments in physical chemistry related to the instrumental techniques – viscometry, conductometry, potentiometry, spectrophotometry, etc. Upon completion of the course, students will be able to handle the relevant laboratory instruments and to know about collection, handling, manipulations and systematic reporting of data, calibration of laboratory equipment and construction of calibration curve. The achieved knowledge will help the students in developing career in chemical and pharmaceutical industries, and to pursue higher studies in different areas of in chemistry.

- 1. Determination of the molar mass of a given polymer.
- 2. Determination of the limit of homogeneous phase in the three component system: chloroform-acetic acid-water.

- 3. Determination of the rate constant and order of $S_2O_8^{2^-}$ in the reaction $S_2O_8^{2^-}_{(aq)} + 2\Gamma_{(aq)} \rightarrow 2SO_4^{2^-} + I_{2(S)}$
- 4. Kinetic studies on the oxidation of ethanedioic acid.
- 5. Determination of the Avogadro constant.
- 6. Studies on the substituent effect on reactivity by measuring the rate of base catalysed hydrolysis of methyl benzoate.
- 7. Determination of the ΔG° , ΔS° , ΔH° and ΔC_p° for the equilibrium reaction $I_2 + \Gamma$ ____ I_3^{-} .
- 8. Determination of the energy of activation for the reaction $5KBr + KBrO_3 + 2H_2SO_4 = 3Br_2 + 3K_2SO_4 + 3H_2O$.
- 9. Studies of adsorption on liquid surfaces by surface tension measurements.
- 10. Verification of the formula of inorganic big molecules, e.g., $KMnO_4$, $K_2Cr_2O_7$ by the ebullioscopic / cryoscopic methods.
- 11. Determination of percentage composition of a binary mixture of nonvolatile nonelectrolyte, e.g., urea, glucose by ebullioscopic / cryoscopic methods.
- 12. Determination of Vant Hoff factor of an electrolyte by ebullioscopic / cryoscopic methods.
- 13. Determination of the dissociation constant of a weak acid (e.g. acetic acid, oxalic acid etc.) near 100°C/0°C by ebullioscopic / cryoscopic methods and estimation of pH of the solution.
- 14. Determination of the hydrolysis constant of a salt conductometrically.
- 15. Determination of activity coefficient conductometrically.
- 16. Kinetic studies on the saponification of an ester conductometrically.
- 17. Determination of the solubility product constant of a suitable salt conductometrically.
- 18. Determination of the standard oxidation-reduction potential of the Fe^{2+}/Fe^{3+} system.
- 19. Determination of the instability constant of the argentamine complex potentiometrically.
- 20. Determination of the hydrolysis constant of a salt potentiometrically.
- 21. Determination of the mean activity coefficient of an electrolyte potentiometrically.
- 22. Determination of the equilibrium constant of $\operatorname{Sn}^{4+} + 2\operatorname{Fe}^{2+} \longrightarrow \operatorname{Sn}^{2+} + 2\operatorname{Fe}^{3+}$ potentiometrically.
- 23. Potentiometric titration of a dibasic acid with NaOH and determination of the first and second dissociation constant of the acid.
- 24. Determination of isobestic point.
- 25. Determination of the indicator constant of an indicator.

- 26. Study of the equilibrium in aqueous solution between ferric nitrate and sodium thiocyanate spectrophotometrically and estimation of stability constant and coordination number of Fe^{3+} .
- 27. Determination of the solubility product constant of Cu(II) iodate spectrophotometrically.

Recommended Books:

- 1. D.P. Shoemaker et al: Experiment in Physical Chemistry
- 2. G.S. Weiss et al: Experiments in General Chemistry
- 3 A. Findlay: Practical Physical Chemistry
- 4. R.C. Das: Experimental Physical Chemistry
- 5. J.N. Gurtu: Advanced Experimental Chemistry
- 6. K.K. Sharma: An Introduction of Practical Chemistry
- 7. J.C. Muhler et al: Introduction to Experimental Chemistry
- 8. J. Rose: A Textbook of Practical Physical Chemistry
- 9. J.B. Yadav: Advanced Practical Physical Chemistry
- 10. Newcomb, Wilson et al: Experiments in Physical Chemistry
- 11. Daniels et al: Practical Physical Chemistry
- 12. Brennan et al: Experiments in Physical Chemistry
- 13. S.R. Palit: Practical Physical Chemistry
- 14. C.D. Hodgman et al: Handbook of Chemistry and Physics
- 15. R.C. West et al: CRC Handbook of Physics and Chemistry
- 16. L.A. Lange: Handbook of Chemistry

Course: Chem 599 Thesis on Physical Chemistry Full Marks: 200 (2.0 unit, 8 credits)

- (i) Thesis : 150 marks
- (ii) Viva-voce: 50 marks

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M.Sc. Examination, 2019 [General Group] M.Sc. Examination, 2020 [Thesis Group]

ORGANIC BRANCH

The Courses and distribution of marks are as follows:

<u>Courses</u>	Course Titles	<u>Units</u>	<u>Credits</u>	<u>Marks</u>
Chem 521F	Organic Reactions and	1.0	4	100
	Stereochemistry			
Chem 522F	Synthetic Organic Chemistry	1.0	4	100
Chem 523F	Advanced Organic Spectroscopy and	1.0	4	100
	Chromatography			
Chem 524F	Macromolecular Chemistry	1.0	4	100
Chem 525F	Bioorganic and Food Chemistry	1.0	4	100
Chem 526F*	Advanced Reaction Mechanism and	1.0	4	100
	Stereochemistry			
Chem 527F*	Organic Pollutants in the	1.0	4	100
	Environment			
Chem 528F*	Biologic Chemistry	1.0	4	100
Chem 521VF	Viva-voce	1.0	4	100
Chem 521L**	Organic Chemistry Practical	2.0	8	200
·	OR			·
Chem 599***	Thesis (Organic / Industrial)	2.0	8	200
	Total	9.0	36	900

- * Students shall have to choose any one out of the three optional courses subject to the approval of the branch.
- ** Laboratory course includes 30% (60) marks for continuous Lab assessment.
- *** Thesis includes 25% marks for oral examination on the thesis.

The M.Sc. Program in Chemistry for General Group shall extend over a period of one academic year and for Thesis Group shall be of two academic years. The final examination on theory courses for both General and Thesis Groups shall be held together at the end of one academic year.

All theory courses include 80% final examination and 20% in-course. The **Final examination** of 80% of each 100 marks (1.0 unit, 4 credits) theory full course shall be of 4 (four) hours duration. In-course comprises of 15% tutorial or terminal and 5% class attendance. The respective class **teachers** of each course shall submit the average marks of in-courses in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last class held. The relevant **examination committee** shall prepare the result by adding the average marks of each in-course to the average marks of each in the final examination of respective course, and send a copy of the average marks of each in-course to the controller of examinations.

The practical course includes 70% practical examination and 30% continuous Lab assessment. The practical examination of 70% of 200 marks (2.0 units, 8 credits) practical course shall be of 24 (twenty four) hours duration (4 days). The students are required to submit a report after each practical class to the class teacher(s) for evaluation. After evaluation the report shall be returned to the students. The class **teacher(s)** shall submit the average marks of all Lab evaluation in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last Lab class held. The examination committee shall send a copy of each of the consolidated **practical** and **Lab evaluation** marks to the **controller** of examinations.

Viva-voce examination (**Chem 521VF**) includes the assessment of the students through oral examination (of all the courses) by the **members** of the relevant examination committee. The **examination committee** shall send a copy of the marks to the **controller** of examinations.

N.B. Students having less than 60% class attendance shall not be allowed to sit for the examination.

Course: Chem 521F Organic Reactions and Stereochemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

Students shall be able to learn recent advances in organic reactions particularly redox and hydrogenation reactions, stereochemistry and skill in asymmetric synthesis. By learning this course students shall be able in designing protocol for the synthesis of specific stereo-regular compounds.

- 1. Alkylation of Active Methylene Compounds (10 Lectures): The formation of enols and enolate anions and their importance, umpolung and its uses in organic transformation, alkylation of relatively active methylene compounds (C-alkylation and O-alkylation), selective alkylation, the formation and alkylation of enamines and dithianes.
- 2. Redox Reactions:

a) Oxidation Reactions (15 Lectures): Oxidation of alcohols with Cr(VI), DMSO, DCC, PCC, Jone's and Collin's reagent, Corey-Kim oxidation, allylic oxidation [SeO₂ and Pb(OAc)₄], peracid and BAIB oxidation, Lemieux, Prevost and Woodward oxidation.

b) Reduction Reactions (15 Lectures): Catalytic hydrogenation, metal hydride reductions, $[\text{LiAlH}_4, \text{LiAlH}(\text{OC}_4\text{H}_9)_3]$, $B_2\text{H}_6$, 9-BBN, DIBAL, NaBH₄, Nacyanoborohydirde, reduction with dissolving metals, hydrazine and its derivatives, Birch reduction, CBS reductions to different organic system.

- **3. Protection and Interconversion of Functional Groups** (10 Lectures): The strategy of using protective groups, its application in the protection of hydroxyl (alcoholic and phenolic), carbonyl, carboxyl, amino and thiol groups. Demerits of protecting group.
- 4. Unusual Optical Activity (15 Lectures): Optical activity due to atoms other than Carbon; N, P, Se, chirality in molecules devoid of chiral center; atropisomerism; nomenclature, synthesis and stereochemistry of biphenyls, allenes, cyclic allenes, spiranes, molecules with planar chirality, stereochemistry of tricovalent carbons; carbonium and carbanions, prostereoisomerism, prochirality and pseudochirality, enantiotopic and diastereotopic ligands and faces. Modern techniques of resolution for racemate.

5. Asymmetric Synthesis and Stereochemistry (15 Lectures): Chirality of conformationally mobile system, conformational stability of substituted cyclohexane and cylodecanes, methods of correlation for configurations. ORD, CD, hydrogen transfer from chiral reducing agents, use of asymmetric MPV reduction to determine the configuration of biphenyl derivatives, use of asymmetric Grignard reagents in creating chiral centers for stereoselective, regeoselective, diastereoselective and enantioselective synthesis, optical purity and enantiomeric excess, chiral catalyst, uses of chiral ligands to organic synthesis.

Recommended Books:

- 1. Adams et al (ed.): Organic Reactions (all volumes)
- 2. H. O. House: Synthetic Application of Organic Reactions
- 3. W. Carruthers: Some Modern Methods of Organic Synthesis
- 4. H. Gilman: Advanced Organic Chemistry, (Vol-I to IV)
- 5. L. F. Fieser and M. Fieser: Introduction to Organic Chemistry
- 6. I. L. Finar: Organic Chemistry Vol. 2
- 7. R. K. J. Mackil and D.M. Smith: A Guidebook to Organic Synthesis
- 8. T. W. Greene: Protective Groups in Organic Synthesis
- 9. L. G. Jr. Wade: Organic Chemistry
- 10 E. L. Eliel, S. H, Wilen and L. N. Mander: Stereochemistry of Organic Compounds

Course: Chem 522F Synthetic Organic Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This advanced course is to provide brief idea on designing organic synthesis and various aspects of quality management of drug and agrochemicals. This course will enable students to know the latest idea available on organometallics and multinuclear heterocycles.

1. Disconnection Approach (13 Lectures): Strategy in organic synthesis; retrosynthesis, one step disconnections, synthon, synthetic equivalent and target molecule, disconnection of simple alcohols, olefins and ketones, two group

disconnections, β -hydroxy carbonyl compounds, α , β -unsaturated carbonyl compounds and 1, 3-dicarbonyl compounds.

- **2.** Multinuclear Aromatic Heterocycles (13 Lectures): General characteristics, preparation and properties; benzo-derivatives of furan, pyrrole, thiophene, indole, acridine, phenathridine and diazanaphthalenes. Synthesis of heterocycles by multicomponent scaffold, one-pot synthesis.
- **3. Polycyclic Aromatic Compounds** (10 Lectures): General characteristics, structure, reactions and synthesis of anthracyclines, tetracyclines, angucyclines, cyclophanes and rotananes.
- **4. Organometallic Chemistry** (13 Lectures): Organo-copper, organo-zinc, organopalladium, organo-silicon, organomagnesim, organoselenium and organo-tin compounds; preparation, properties and synthetic uses, homogeneous catalyst to different organic transformations.
- **5. Agrochemicals** (10 Lectures): A brief introduction of organochlorine and organophosphosphorus compounds, carbamates, dithiocarbanic acid derivative as agrochemicals, cause of resistance in the insect system, syntheses of i) herbicides: vegadex, avadex, eptam and carbyne ii) fungicides:vapam, nabam and zineb iii) insecticides: sevin and furadan. Uses of pheromones as insect repellant.
- 6. Some Important Drugs (13 Lectures): Principle of combinatorial synthesis, its advantages and limitations, syntheses of salbutamol, trimethoprime, indomethacin, acetazolamide, naproxen and tolmetin sodium.
- 7. Quality Control Assurance and Validation (8 Lectures): Importance of pharmaceutical analysis for the quality control of drugs, concept of quality assurance, selection and testing of major raw materials, quality management consideration, comparative Q_C/Q_A method development and validation. Process development of existing products facility.

- 1. E. S. Gould: Mechanism and Structure in Organic Chemistry
- 2. R. T. Morrison and R. N. Boyd: Organic Chemistry
- 3. S. Warren: Disconnection Approach.
- 4. P. Simpson: Organometallic Chemistry of the Main Group Elements.
- 5. A. Kar: Medicinal Chemistry.
- 6. A. Burger: Medicinal Chemistry and Drug Discovery (Vol. I and II)
- 7. S. F. Dyke: Advances in Heterocyclic Chemistry
- 9. Atta-ur-Rahman and Zhahir Shah: Stereoselective Synthesis in Organic Chemistry.
- 10. D. A. Skoog: Principle of Instrumental Analysis.

Course: Chem 523F Advanced Organic Spectroscopy and Chromatography Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This advanced course addresses various aspects of spectroscopic chemical analyses and separation techniques strongly bonded to both research and industry.

1. UV-Vis and ESR Spectroscopy (15 Lectures):

a) Theory and experimental techniques of UV, application in the identification of organic molecules, Woodward, Woodward-Fieser and Nielsen's rules for the determination of λ_{max} to different organic molecules.

b) Introduction and basic principle of ESR, sensitivity, saturation, spin lattice relaxation, Breit-Rabi equation, operation of ESR spectrometer, components line position, isotropic ESR spectra, hyperfine coupling spectra and its application.

- **2. Infrared Spectroscopy** (7 Lectures): Basic principle, modes of vibrations, applications, wave numbers for different functionality, IR for flexible molecules and stereo-chemical aspects.
- 3. **Raman Spectroscopy** (8 Lectures): Introduction and basic principle, Raman shifts, stokes and anti-stokes line, Rayleigh line, kinds of Raman spectra, instrumentation, chemical and electro-magnetic enhancement, Raman selection rules and insensitivities, application to organic molecules, advantages of Raman spectra.
- 4. NMR Spectroscopy (20 Lectures): ¹H, ¹³C, ³¹P, ¹⁹F NMR spectroscopy; preamble, principles of NMR, situation for other nuclei, continuous wave and pulsed NMR experiments, FID and processing FID, relaxation, chemical shifts and factors influencing it, origin of coupling, long-range coupling, coupling constant, signal-to-noise ratio (SNR), integration of signals, NOE, SPI, INDOR, DEPT and APT techniques; 2D-NMR, basics of 2D NMR, general experimental scheme for 2D NMR, COSY, NOESY, HETCOR; extensive application of NMR to bigger organic molecules.
- **5.** Mass Spectroscopy (20 Lectures): Base peak, molecular ion peak, metastable peak and their utility, fragmentation patterns to various organic molecules, description of HRMS, LIMA, SIMS, MALDI and FAB techniques in mass spectroscopy, structural study of simple and complex organic compounds and application to macromolecules, GC-MS, LC-MS; principle and instrumentation of GC and LC, combined techniques (GC-MS, LC-MS) for chemical analyses.
- 6. Chromatography (10 Lectures): Column chromatography and its basic principle, flash and vacuum liquid chromatography, gas chromatography; GSC, GLC, HPLC with chiral column.

Recommended Books:

- 1. P. S. Sindhu: Molecular Spectroscopy
- 2. J. D. Graybeal: Molecular Spectroscopy
- 3. R. K. Harris: Nuclear Magnetic Resonance Spectroscopy
- 4. D. L. Pavia, G. M. Lampman and G. S. Kriz and J. A. Vyuvan: Introduction to Spectroscopy
- 5. Y. R. Sharma: Elementary Organic Spectroscopy; Principles and Chemical Application
- 6. H. Friebolin: Basic One- and Two-dimentional NMR Spectroscopy
- 7. H. C. Hill: Mass Spectroscopy
- 8. Gray D. Christian: Analytical Chemistry
- 9. H. Gunther: NMR Spectroscopy
- 10. J. K. M. Sanders and B. K. Hunter: Modern NMR Spectroscopy
- 11. R. J. Abraham and P. Loftus: Proton and Carbon-13 NMR Spectroscopy
- 12. I. D. Campbell and R. A. Dwek: Biological Spectroscopy
- 13. D. Williams and L. Fleming: Spectroscopic Methods in Organic Chemistry
- 14. V. R. Dani: Organic Spectroscopy
- 15. P. S. Kalsi: Spectroscopy of Organic Compounds
- 16. Silverstein et al: Spectrometric Identification of Organic Compounds

Course: Chem 524F Macromolecular Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

On completion of this course students shall be able to become intimate with recent methods and chemistry of polymerization, polymer stability, and their industrial applications. Students shall also be able to design recipe for the fabrication of polymer materials to develop new products with scope for specific application.

1. General Idea on Polymer (10 Lectures): Introduction; polymer, monomer, oligomer, repeating units, structure of polymer molecules based on configuration and conformation, classification of polymers, intermolecular forces, biological and industrial importance of polymers, end group analysis, polymer solutions;

thermodynamics of polymer dissolution, size and shape of macromolecules in solution.

- 2. Types and Mechanism of Polymerization (15 Lectures): Types of polymerization reaction; chain polymerizations (free radical, ionic and coordination), step polymerizations (poly-condensation, poly-addition and ring-opening), mechanism of each polymerization, kinetics, chain length and degree of polymerization, initiation and initiator efficiency in free radical polymerization, gel effect, inhibition and retardation, elementary idea on oxidative and atom transfer radical polymerizations, nitroxide mediated controlled polymerization.
- **3. Stereochemistry of Macromolecules** (10 Lectures): Stereo-regularity of polymers, stereochemical control polymerization by Zieglar Natta and MAO catalyst, especially in polymerization of propylene, butadiene, isoprene etc.
- **4. Copolymers** (10 Lectures): Classification of copolymers, structure of copolymers, preparation of block and graft copolymers, kinetics of free radical copolymerization, reactivity ratio and its measurement, significance of reactivity ratio, copolymer equation for ideal and alternating copolymer.
- **5. Polymer Colloids** (10 Lectures): Latex, chemistry of polymer colloid formation; brief introduction on emulsion and dispersion polymerizations, general idea on solution, bulk and suspension polymerizations, colloidal stability, applications of polymer colloids in paper, adhesives, coating and other industries.
- **6. Polymer Degradation** (15 Lectures): Introduction, types of degradation; thermal, mechanical, oxidative, hydrolytic and photodegradation, factors affecting thermal degradation, degradation by high energy, ultrasonic wave and bacteria.
- 7. Monomers and Related Petrochemicals (10 Lectures): Petrochemicals, classification of petrochemicals, distillation products from petroleum, reactions of alkanes, alkenes and aromatics, solvents and specific applications, synthesis of butadienes, acrylonitrile, acrylic acid, styrene, glycerin and surfactant.

- 1. Royal Dutch (Shell Company): The Petroleum Handbook
- 2. W. L. Nelson: Petroleum Refining Engineering
- 3. R. N. Shreve: Chemical Process Industries
- 4. B. K. Sharma: Industrial Chemistry
- 5. V. R. Gowariker et.al: Polymer Science
- 6. G. Odian: Principles of Polymerization
- 7. Fred W. Billmeyer Jr.: A Textbook of Polymer Science
- 8. Robert M. Fitch: Polymer Colloids: A Comprehensive Introduction

Course: Chem 525F Bioorganic and Food Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course contributes important features to chemical biology, enzymology, genetics, physiology, immunology, pharmacology and computational aspects of drug designing, their structure-activity relationship, nutrition, agriculture, food additives and preservation technologies; practically all of the primary specialties on the life sciences aiming at the development of drug and medicinal products.

- **1. Enzyme Catalyzed Reactions** (12 Lectures): Definition of enzyme, coenzyme, holoenzyme and apoenzyme, enzyme properties, enzyme inhibitors, origin of enzyme specificity, enzyme kinetics, enzyme-catalyzed interconversion of acetaldehyde and ethanol, ester and carboxylic acid, identification of functional groups essential for catalysis, factors affect the catalytic efficiency of enzymes, reaction mechanism at enzyme active site; action of chymotrypsin on dipeptide, hydrolysis of peptides with carboxypeptidase.
- 2. Molecular Recognition (8 Lectures): Introduction, recognition of guests by synthetic hosts, natural hosts, ionophores; molecular recognition by an enzyme, catalytically active antibodies, nucleic acids, cryptands, spherands, epitope and antigen.
- **3. Biomolecules** (8 Lectures): Occurrence, structure, stereochemistry and biological properties of lipids, prostaglandins and nucleic acids, biosynthesis of prostaglandins (e.g., PGI), nucleosides (e.g., adenosine, thymidine etc.), nucleotides and nucleic acids (e.g., RNA, DNA).
- 4. Receptors and Drug Action (8 Lectures): Role of receptors, neurotransmitter, ecosanoids, cannabinoid molecules, design of agonis, antagonis, receptor, biological response, drugs action on DNA, quantitative structure activity relationship (QSAR).
- **5.** Nutritional Aspects of Foods (12 Lectures): Function of human organs (siver, heart), function of fats, phospholipids and cholesterol, essential fatty acid deficiency in human beings, effect of excess essential fatty acids, fatty liver diseases and lipotropism, dietary lipids and their relation to the causation of atherosclerosis and ischaemic heart disease, protein efficiency ratio (PER), digestibility coefficient, biological values of protein, net protein utilization (NPU), net protein ratio (NPR), effect of amino acid imbalance and amino acid toxicity.
- 6. Food and Food Additives (10 Lectures): Different classes of foods; types of food additives (polysorbate 60, dimethyl pyrocarbonate), effect on stability of nutrient,

direct and indirect effect of food additives on health; chemical changes in food during storage at room temperature and at frozen state.

- **7.** Food Adulteration (10 Lectures): Definition of adulterated food, common adulterants in different foods; contamination of foods with toxic chemicals, pesticides and insecticides; bacterial and fungal contamination of food, effect of radiation in food.
- 8. Food Preservation and Processing (12 Lectures): Detoriation factors and their control, chemical preservation, heat processing, protection by packaging material, fruit/vegetable specific preservation; fresh and semi processed storage, juice technology, sugar preserve technology; jam, jelly, etc., pickles and sauerkraut technology, mango, guava and banana processing technologies.

Recommended Books:

- 1. Seyhan Ege: Organic Chemistry Structure and Reactivity.
- 2. R. K. Bakiaski: Modern Biochemistry
- 3. Murray et al.: Harper's Illustrated Biochemistry
- 4. U. Satayanarayana: Biochemistry (2nd ed.)
- 5. David L. Nelson and Michael M. Cox: Lehninger's Principle of Biochemistry
- 6. Tortora, Funke and Case: Microbiology: An Introduction
- 7. Graham L. Patrick: An Introdction to Medicinal Chemistry
- 8. M. Swaminathan: Advanced Text book on Food and Nutrition, Vol. I and II
- 9. M. Swaminathan: Essential of Food and Nutrition, Vol. I and II

Course: Chem 526F Advanced Organic Reactions Mechanism and Stereochemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course focuses on advanced mechanistic- and stereochemistry. This course also gives opportunity to acquire preliminary ideas on green chemistry with new and modern approaches of chemical synthesis, catalysis, process chemistry, nanochemistry, ways for preventing pollution and reducing consumption of non-renewable resources.

1. Principles of Reactivity and Methods of Determination of Reaction Mechanism (20 Lectures): Consecutive reaction, the steady-state approximation, Hammond postulate, Hammond potential energy surface model, reactivityselectivity principle, Arrhenius equation, Eyrring equation, linear free energy relationship (LFER), resonance and field effects, steric effects, effect of structure on activity, Hammett and Brönsted type LFER, limitation and modification of Hammett equation; Taft, Yukwa-Tsuno equation.

- 2. Click and Cascade Reactions (15 Lectures): Definition, background, advantages and applications of click chemistry, click reaction in cycloaddition, thiol-ene reaction, azide-alkyne Huisgen cycloaddition, olefin based organic synthesis, click reaction in polymer science, nanostructure synthesis and surface modification, click chemistry in water. Definition and examples of cascade reactions, mechanisms.
- **3.** Green Techniques in Organic Synthesis (15 Lectures): Reactions in water, ionic liquids, zeolites, microwave heating, ultrasound in organic reactions, supercritical liquids, organo-catalysts and phase transfer catalysts. Uses of enzymes in organic reactions.
- 4. Mechanism of Named Organic Reactions (15 Lectures): Shapiro reaction, Sonogashira, Heck, Hosomi-Sakurai, Stille coupling, Kumada coupling, Nigishi, Suzuki Coupling, B. Sharpless, Baylis-Hillmann, Biginelli reaction, Gewald, Passerini, Corey-Winter olefination and Pauson-Khand reaction.
- 5. Pericyclic Reactions (15 Lectures): Cycloaddition and cycloreversion, electrocyclic, chelotropic reaction, sigmatropic rearrangement, tandem reaction, their stereochemical considerations, component analysis (allowed or forbidden), Diels-Alder reaction to bigger molecule synthesis, Cope-Claisen rearrangement and their orbital interaction analysis.

- 1. R. Adams et al: Organic Reactions (all volumes)
- 2. Alder, Baker and Brown (Wiely and Sons): Mechanism in Organic Chemistry
- 3. Ian Fleming (Wiely and Sons): Frontier Orbital and Organic Reactions
- 4. H. Gilman: Advanced Organic Chemistry, (Vol-1 to IV)
- 5. L. F. Fieser and M. Fieser: Introduction to Organic Chemistry
- 6. Neil S. Issac (Longman): Physical Organic Chemistry
- 7. T.W. Greene: Protective Groups in Organic Synthesis
- 8. J. March: Advanced Organic Chemistry
- 9. W. Carruthers: Some Modern Methods of Organic Synthesis
- 10. H. O. House: Synthetic Application of Organic Reactions
- H. C. Kolb, M. G. Finn and K. B. Sharpless: "Click Chemistry: Diverse Chemical Function from a Few Good Reactions". <u>Angewandte Chemie international</u> 2001, 40 (11): 2004–2021.

Course: Chem 527F Organic Pollutants in the Environmental Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

This course elaborately discloses the current chemical hazards, toxic materials, biological injury to health and has given some guidelines on remedial methods to minimize the detrimental effects of these hazards.

- 1. Chemical Pollutants in the Environment (8 Lectures): Primary and secondary, natural, manmade, municipal, agricultural and industrial pollutants, bioaccumulation, biomagnifications, biodegradation and biotransformation.
- **2.** Pollution by Hydrocarbons (15 Lectures): Petroleum and acuatic organism, biphenyl, polychlorinated biphenyls (PCBs), physical and chemical properties, environmental distribution and behavior, polycyclic aromatic hydrocarbons (PAHs).
- **3. Pollutant from Industries** (15 Lectures): Polymer and plastic, soap and detergent, chemical and pharmaceutical, pulp and paper industries, abatement procedures for the reduction of pollution from different industries.
- 4. Organic Pollutants in Vegetables, Fruits, and Other Food Materials (15 Lectures): Insecticide, herbicide, fungicide and their effects on environment and human health, mechanism of action of metabolism of pesticide in biological system, natural and artificial contaminants in food, synthetic food color, dye, preservative, ripening agents, detoxification and their metabolites in the environment.
- **5. Fertilizers** (10 Lectures): Nitrogenous, phosphatic and NPKS fertilizers, environmental implication of fertilizer.
- 6. Waste Management and Integrated Paste Management (10 Lectures): Appropriate disposal by proper chemical and biological treatment of domestic, industrial and medical wastes, definition, key components of IPM, pest control technique, reduction of pollutants.
- **7. Organometallic Pollutants** (7 Lectures): Nature, stability and sources of organometallic compounds; organomercury, organolead, organotin, organoarsenic compounds; behavior in water, air, soil and sediments.

- 1. Stanley and Manahan: Environmental Chemistry (4th ed.)
- 2. A. K. Dey: Environmental Chemistry
- 3. Stoker and Seager: Environmental Chemistry
- 4. Khopkar (Wielly Estern Ltd.) : Environmental Pollution Analysis
- 5. T. R. Crompton: Determination of Organic Substances in Water (Vol II)
- 6. B. C. Rana: Pollution and Biomonitoring
- 7. Roy Chester: Marine Geochemistry
- 8. R. Haque: Toxic Chemicals

Course: Chem 528F Biologic Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

At the end of the course the students will know the physiological functions and consequence of the deficiency of some special biomolecules, such as, lipids involved in cell functions, carbohydrates for cell organelles and protein synthesis, amino acids and proteins related to nutrition.

- 1. Lipids of Physiologic Significance (15 Lectures): Classification of lipids, physiologic functions, unsaturated fatty acids, ω -fatty acids, eicosanoids, modifications, classes and functions, phospholipids and glycosphingo-lipids and their functions. Free radical reactions in lipids, role of anti-oxidents in protecting lipids.
- 2. **Carbohydrates in Physiologic Significance** (15 Lectures): Glycogens, ribose and deoxyribose, glactose in milk synthesis, glycoproteins, glycolipids, proteoglycans. Diabetes mellitus, glactosemia and glycogen shortage diseases, lactose intolerance and glycemic index.
- 3. **Biologic Oxidation** (13 Lectures): Redox potential and flow of electrons in biologic systems, enzyme involved in oxidation and reductions for the biologic system. Action of oxydases, NAD and P-450 and superoxide dismutase.
- 4. **Metabolism of Protein and Amino Acids** (12 Lectures): Nutritionally essential amino acids, identification, key role of trans-aminases in amino acid metabolism, hydroxyl proline and hydroxyl lysine in protein formation, causes of severe deprivation of Vit-C, consequence of its nutritional disorder. Selenocystein and mammalian proteins.
- 5. Catabolism of Proteins and Amino Acids (15 Lectures): Protein turnover, ATP dependent and ATP independent turnover of proteins, proteins turnover in mammals, in birds and in fishes. Formation of urea during N-catabolism in human. Metabolic disorder associated with catabolism.
- 6. **Chemistry of Aging** (10 Lectures): Wear and tear theories of aging, common environmental factors to damage of DNA and proteins. Bases of nucleotide are vulnerable to damage. Mitochondrial and nuclear genomes, ROS (reactive oxygen species), mechanism of cell repairing by ROS.

- Robert K. Murray, D. A. Bender and K.M. Botham: Herper's Illustrated Biochemistry (29th Edition)
- 2. David L. Nelson and Michael M. Cox : Lehninger's Principle of Biochemistry

Course: Chem 521L Organic Chemistry Practical Examination: 24 hours (4 days) Marks: 200 (2 units, 8 credits)

(i) Experiment: 140 (ii) Continuous Class Evaluation and Class Record: 60

Intended Learning Outcomes (ILO)

On completing this advanced practical course the students shall be able to synthesize organic compounds via multi-step synthesis, separate and purify intermediates by TLC, column chromatography and paper chromatography. The students shall also gain practical knowledge on how to use advanced tool for the characterization of synthesized compounds.

- 1. Crystallization, extraction, distillation and drying of organic compounds / reagents.
- 2. Fractional distillation: ethanol from sugar; extraction from solution.
- 3. Multistep organic synthesis: a) synthesis of nitrophenols, paracetamol b) preparation of sulphanilamide and other sulphur drugs c) synthesis of benzyllic acid from benzoin via benzil formation d) preparation of acridone from anthranilic acids e) synthesis of methyl orange from sulphanilic acid (some other synthesis may also be included if facilities are made available).
- 4. Preparation of ketals, esters; fats and detergents, reactions of aldehydes and ketones and heterocyclic compounds like coumarins, beta keto esters, cyclohexene from cyclohexanol.
- 5. Chromatographic method: TLC, column chromatography, paper chromatography.
- 6. Assay of drugs and raw materials: a) ephedrine hydrochloride b) penicillin/ ampicilline capsule c) cotrimoxazole tablet/syrup d) aspirin tablet etc. (some other suitable compounds if they are available. Uses of UV-Vis and IR spectrometers)
- 7. Resolution of recemic compounds (acids/bases).
- 8. Oxidation: selective oxidation; oxidation of primary and secondary alcohol and aldehyde.
- 9. Reduction: sodium borohydride reduction of benzil and other compounds containing carbonyl groups.
- 10. Hydroboration: hydroboration of unsaturated hydrocarbons.
- 11. Phase transfer catalysis: use of PTC in different types of reactions.
- 12. Reaction kinetics: hydrolysis of tert-butyl chloride etc.

Course: Chem 599 Thesis on Organic/Industrial Chemistry Marks: 200 (2 units, 8 credits)

- (i) Thesis: 150 marks
- (ii) Thesis defence: 50 marks

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M.Sc. Examination, 2019 [General Group] M.Sc. Examination, 2020[Thesis Group]

INORGANIC BRANCH

The courses and distribution of number are as follows:

<u>Courses</u>	Course Titles	<u>Units</u>	<u>Credits</u>	<u>Marks</u>		
Chem 531F	Organometallic Chemistry	1.0	4	100		
Chem 532F	Bioinorganic Chemistry	1.0	4	100		
Chem 533F	Inorganic Materials	1.0	4	100		
Chem 534F	Analytical Chemistry	1.0	4	100		
Chem 535F	Homogeneous and Heterogeneous	1.0	4	100		
	Catalysis					
Chem 536F	Environmental Chemistry	1.0	4	100		
Chem 531VF	Viva-voce	1.0	4	100		
Chem 531L*	Inorganic Chemistry Practical and Project	2.0	8	200		
OR						
Chem 599**	Thesis / Dissertation on topics of	2.0	8	200		
	Inorganic Chemistry					
!	Total	9.0	36	900		

* Laboratory courses includes 30% (60) marks for continuous Lab assessment.

** Thesis includes 25% (50) marks for oral examination on the thesis.

The M.Sc. Program in Chemistry for General Group shall extend over a period of one academic year and for Thesis Group shall be of two academic years. The final examination on theory courses for both General and Thesis Groups shall be held together at the end of one academic year.

All theory courses include 80% final examination and 20% in-course. The **Final examination** of 80% of each 100 marks (1.0 unit, 4 credits) theory full course shall be of 4 (four) hours duration. In-course comprises of 15% tutorial or terminal and 5% class attendance. The class **teachers** of each course shall submit the average marks of in-courses in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last class held. The relevant **examination committee** shall prepare the result by adding the average marks of each in-course to the average marks of each in the final examination of respective course, and send a copy of the average marks of each in-course to the controller of examinations.

The practical course includes 70% practical examination and 30% continuous Lab assessment. The practical examination of 70% of 200 marks (2.0 units, 8 credits) practical course shall be of 24 (twenty four) hours duration (4 days). The students are required to submit a report after each practical class to the class teacher(s) for evaluation. After evaluation the report shall be returned to the students. The class **teacher(s)** shall submit the average marks of all Lab evaluation in a sealed envelope to the **chairman** of the relevant **examination committee** within three weeks from the last Lab class held. The examination committee shall send a copy of each of the consolidated **practical** and **Lab evaluation** marks to the **controller** of examinations.

Viva-voce examination (**Chem 531VF**) includes the assessment of the students through oral examination (of all the courses) by the **members** of the relevant examination committee. The **examination committee** shall send a copy of the marks to the **controller** of examinations.

*Students having less than 60% class attendance shall not be allowed to sit for the examination.

Course: Chem 531F Organometallic Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

Upon studying the course the students will learn to describe the synthesis, structure and bonding of organometallic compounds of $\eta^l - \eta^8$ systems as well as organometallic compounds of main group elements. They will also learn various types of organometallic reactions, synthesis, structure and bonding of metallocenes with special reference to ferrocene.

- 1. **Preliminary Idea of Organometallic Chemistry (7 Lectures):** Introduction, classification, nomenclature and characteristics of organometallic compounds, structure, bonding and general aspects.
- 2. Organometallic Compounds of Main Group Elements (10 Lectures): Introduction, general characteristics, stability of organometallic compounds, preparation route for metal-carbon bonds: oxidative-addition reactions, metal-metal exchange reactions (transmetallation), carbanion-halide exchange reactions, alkylation (or arylation) reactions, reactions with protic reagents, reactions with hydridic hydrogen, redistribution reactions, pyrolysis and complex formation.
- 3. Organometallic Compounds of Transition Metals (10 Lectures): Introduction and nature of bonding, insertion reactions, elimination reactions, cyclometallation reactions, metal atom reactions, properties of σ -hydrocarbyls of transition metals: general characteristics, chemical reactions, bonding and structure, thermal stability and decomposition pathways.
- 4. Types of Organometallic Reactions (18 Lectures):
- (a) **Oxidative addition reactions:** Reaction with protons, reactions forming metalcarbon bonds, reactions with hydrogen bonds.
- (b) **Reductive-eliminations:** Reactions forming carbon-carbon bonds, reactions forming carbon-hydrogen bonds.
- (c) **Insertion reactions:** Migratory insertions, acyl formation, stereochemistry at the metal and alkyl carbon.

- (d) Reformatsky and Simmons-Smith reactions, oxymercuration-demercuration of alkenes and carbene transfer reactions, hydrosilation of alkenes, dimerization and polymerization of alkenes and alkenes and alkene metatesis.
- 5. π -Bonded Organometallics (20 Lectures):
- (a) Chemistry of $\eta^1 \eta^8$ transition metal complexes (10 Lectures): Preparations, properties and bonding.
- (b) Metallocenes: Preparation, electronic structure and bonding, physical properties, reactions, general aspects. Ferrocene: comparative reactivities of ferrocene and benzonoid aromatics, mechanism of electrophilic substitutions, mechanism of the arylation reactions.
- (c) η^6 -Arene metal complexes: Synthesis, general characteristics, chemical reactivities, structure and bonding.
- 6. Biological Applications and Environmental Aspects of Organometallic Compounds (15 Lectures): Introduction, organometallic compounds in medicine, agriculture and horticulture, and in industry; environmental aspects of organometallic compounds.

- 1. Parcell and Kotz: Inorganic Chemistry
- 2. Cotton and Wilkinson: Advanced Inorganic Chemistry, 5th Edn. (1980)
- 3. J.P. Collman and L.S. Hegedus: Principles and Applications of Organo-transition Metal Chemistry
- 4. J.E. Huheey: Inorganic Chemistry: Principles of Structure and Reactivity
- 5. J.D. Atwood: Inorganic and Organometallic Reaction Mechanism
- 6. W.U. Malik G.D. Tuli and R.D. Madan: Selected Topics in Inorganic Chemistry
- 7. S.Z. Haider: Selected Topics in Inorganic Chemistry
- 8. D.L. Pavia, G.M. Lavepman and G.S. Kriz: Introduction to Spectroscopy (Saunders)
- 9. R. C. Mehrotra and A. Singh: Organometallic Chemistry: A Unified Approach, 2nd Edn. (1991)

Course: Chem 532F Bioinorganic Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

The course is designed to develop the concepts of bioinorganic chemistry with emphasis on the roles of transition metals in biology and medicine. The course focuses on structure-activity relationship of some biomolecules including respiratory proteins, some metalloenzymes, metal ion transport and storage, nitrogen fixation and ironsulfur proteins.

1. **Background** (10 lectures):

a) Essential amino acids, amino acids with (nonpolar, uncharged polar and charged polar) side chains, structure of proteins, peptide bond, binding sites in peptide, enzymes and metalloenzymes.

b) Nucleosides, nucleotides and nucleic acids, structure of DNA, RNA and ATP. Preliminary idea about blood, plasma, the cell (structural and functional unit), eukaryotic cell, plasma membrane, protoplasm, nucleus, mitochondria, lysosomes, ribosomes, endoplasmic reticulum, Golgi complex, cytoskeleton, structure of prokaryotic cell, membrane structure.

- 2. **Essential Trace Elements** (5 lectures): Classification, concept of essentiality, evolution and working system, essential ultra-trace metals and nonmetals.
- 3. **Respiratory Proteins** (15 lectures): Properties of respiratory pigments– a comparison; myoglobin (Mb) and hemoglobin (Hb) (structure and functions), oxygenation reactions, structure function relationship, structural models for dioxygen binding, cooperativity of hemoglobin.

Structural studies of hemerythrin and hemocyanin (Hc), oxygenation curves for Mb, Hb and Hc. Bohr effect, dissociation and association of hemocyanin.

- 4. Metalloenzymes and Metallobiomolecules (20 lectures):
 - (a) Biological redox reactions, types of heme, cytochromes (cytochrome c, cytochrome c oxidase), cytochrome P-450 enzyme. Superoxide and bovine superoxide dismutase, superoxide toxicity, structure of Cu-, Zn-SOD. Enzymatic activity and mechanism, peroxidase and catalase, blue and non-blue Cu-proteins.

- (b) Biochemistry of zinc: Carboxypeptidases, CPA- structure, mechanism of action, specificity of enzymatic reaction, carbonic anhydrase- structure, metallocarbonic anhydrases, mechanism of action, inhibition, kinetic studies.
- c) Biochemistry of cobalt: Vitamin B_{12} sources, structure, functions and its derivatives.
- d) Biochemistry of magnesium: Chlorophyll- classification, structure and function.
- 5. Metal Ion Transport and Storage (10 lectures):

Iron storage and transport: Transferrin, ferritin, synthetic iron-oxo aggregates.

Iron transport in microbes: Siderophores (hydroxamate, phenolate), models for siderophores.

Other storage and transport system: Ceruloplasmin and serum albumin, metallothioneins and phytochelatins.

6. Nitrogen Fixation and Iron-Sulphur Proteins (10 lectures):

Nitrogen fixing microorganisms, nitrogenase (reactivity and redox properties), postulated mechanisms for nitrogen fixation, reduction mechanism involving nitride and diazene intermediate, *in vitro* nitrogen fixation, dinitrogen complexes and their reactivity.

Rubredoxin, ferredoxins, high-potential iron-sulphur proteins (HiHIPs).

- 7. Metals and Coordination Compounds in Medicine (10 lectures):
 - a) Chelation therapy: Dimercaprol, pencillamine, polyaminopolycarboxylic acids, aurinetricaboxylic acid, desferrioxamine, cryptates.
 - b) Gold compounds and rheumatoid arthritis, lithium and mental disorder, arsenicals.
 - c) Mutagens and carcinogens, anticancer drugs such as platinum and gold complexes, metallocene and their halides.
 - d) Antimicrobial agents.

- 1. K. H. Reddy: Bioinorganic chemistry
- 2. I. Bertini, H.B. Gray, S.J. Lippard, and J.S.Valentine: Bioinorganic Chemistry
- 3. Cotton and Wilkinson: Advanced Inorganic Chemistry, 5th Edn. (1980)
- 4. Counther L. Eichhorn: Inorganic Biochemistry, (edited) Vol. I and II

- 5. J.E. Huheey: Inorganic Chemistry: Principles of Structure and Reactivity
- 6. A.C. Deb: Fundamentals of Biochemistry
- 7. K.F. Purcell and J.C. Kotz: Inorganic Chemistry
- 8. M.N. Hughes: The Inorganic Chemistry of Biological Processes
- 9. R.J.P. Williams and De Silva: New Trends in Bioinorganic Chemistry
- 10. E. Ochiai: Bioinorganic Chemistry
- 11. David R. Williams, (Edited) : An Introduction to Bioinorganic Chemistry
- 12. R.W. Hay: Bioinorganic Chemistry
- 13. D.M. Taylor and D.R. Williams: Trace Element, Medicine and Chelation Therapy

Course: Chem 533F Inorganic Materials Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

The course focuses on the properties and application of functional inorganic materials. It includes the bonding of materials, crystal systems and characterization of solid materials with instrumental techniques. Emphasis has been given on the physical properties of materials, performance of materials and specialty materials such as superconductors, liquid crystals and nanomaterials.

- 1. **Introduction to Materials Science and Engineering (8 Lectures):** Materials and civilization, types of materials, materials and engineering, structure, properties, performance.
- 2. **Crystals (Atomic Order) (10 Lectures):** Crystalline phases, cubic structures, noncubic structures, polymorphism, unit-cell geometry, crystal directions, crystal planes .
- 3. Characterisation of Solid Materials (12 Lectures):

- a) X-ray diffraction: Structure determination from powder patterns, influence of crystal symmetry and multiplicities on powder pattern, limitation of powder methods, single crystal X-ray method.
- b) Neutron diffraction: Neutron diffraction, applications, merits and limitations.
- c) Electron Microscopy: Electron diffraction applications, transmission electron microscopy (TEM), scanning electron microscopy (SEM), scanning tunneling microscopy (STM), analytical electron microscopy and atomic force microscopy (AFM).
- 4. **The Physical Properties of Materials (8 Lectures):** Density, thermal properties, diffusion, electrical properties, magnetic properties, dielectric and optical properties.
- 5. **Performance of Materials in Service (10 Lectures):** Service performance, corrosion reactions, corrosion control, delayed fracture, performance of metals at high temperatures, service performance of polymers, performance of ceramics at high temperatures.
- 6. **Superconductors (8 Lectures):** Superconductivity, theories of superconductivity, introduction of low T_c and high T_c superconducting materials, applications, recent development of superconducting materials.
- 7. Liquid Crystals (10 Lectures): Classification of liquid crystals and their possible phase transitions, chemical structure elements in liquid crystals, application of liquid crystals.
- 8. Nanomaterials and Nanotechnology (14 Lectures): Concepts of nanoscale, nanoscience, nanotechnology and nanochemistry. Classification of nanomaterials, physical and chemical properties of nanostructured materials. General synthetic approaches of nanomaterials (top-down and bottom-up approaches). Special nanomaterials— carbon fullerens, carbon nanotubes, graphene, silicon nanomaterials, micro- and mesoporous materials; applications of nanomaterials.

Recommended Books:

1. Lawrence H. Van Vlack: Elements of Materials Science and Engineering

- 2. R.E. Smallman and R.J. Bishop: Metals and Materials
- 3. O.P. Khanna: Material Science and Metallurgy
- 4. A.R. West: Solid State Chemistry and its Applications
- 5. A.K. Cheetham and P. Dey: Solid State Chemistry Techniques
- 6. A.R. West: Basic Solid State Chemistry
- 7. W. D. Callister. Jr.: Materials Science and Engineering- An Introduction
- 8. C.E. Hall: Introduction to Electron Microscopy
- 9. P.J. COllings and M. Hird: Introduction to liquid crystals: Chemistry and Physics
- 10. Narendra Kumar and Sunita Kumbhat: Essentials in Nanoscience and Nanotechnoloty
- 11. Sulabha K. Kulkarne: Nanotechnology: Principles and Practices
- 12. Zhen Guo and Lin Tan: Fundamentals and Applications of Nanomaterials

Course: Chem 534F Analytical Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

The course provides the knowledge of analytical instrumentation including spectroscopy (Raman, ESCA, XPS, AES, SIMS and RBS), electrogravimetry, coulometry, voltammetry and thermogravimetry. The students will learn to apply these instrumental techniques in the chemical analysis and chemical problems.

- 1. Sampling (10 Lectures): Water, air and soil sample processing, trace analysis.
- 2. **Atomic Spectroscopy** (10 Lectures): Absorption, emission and fluorescence methods: theory, measurement, interference and applications.
- Raman Spectroscopy: (6 Lectures): Theory of Raman spectroscopy, excitation of Raman spectra, mechanism of Raman and Rayleigh scattering, wave model of Raman and Rayleigh scattering, intensity of normal Raman peaks, Raman depolarization ratios, instrumentation and applications.

4. Surface Characterization by Spectroscopy (8 Lectures):

Electron spectroscopy for chemical analysis (ESCA), X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), secondary-ion mass spectrometry (SIMS) and Rutherford backscattering spectroscopy (RBS).

- 5. **X-ray Spectroscopy** (10 Lectures): Absorption, emission, diffraction and fluorescence.
- 6. Electrogravimetry and Coulometry (8 Lectures): Theory, instruments and applications.
- 7. **Voltammetry** (12 Lectures): Theory of classical voltammetry, modified voltammetric methods: pulse, cyclic and stripping voltammetry, measurement and applications.
- 8. **Thermal Analysis** (8 Lectures): Differential thermal analysis and differential scanning calorimetry, thermogravimetry and thermometric titrations.
- 9. **Radiochemical methods** (8 Lectures): Radioactive nuclides, counting statistics, instrumentations, neutron activation and isotope dilution methods: principles and applications.

- 1. D. A. Skoog, D. M. West, F.J. Holler and S. R. Crouch: Fundamentals of Analytical Chemistry (9th Ed.)
- 2. D. A. Skoog, F. J. Holler and S. R. Crouch: Principles of Instrumental Analysis (6th Ed.)
- 3. Willard, Merritt, Dean and Settle: Instrumental Methods of Analysis (6th Ed.)
- 4. Bassett, Danney, Jeffery and Mendhams: Vogel's Textbook of Quantitative Inorganic Analysis
- 5. Pavia, Lampman and Kriz: Introduction to Spectroscopy
- 6. L.R. Faulkner and A.J. Bard: Electrochemical Methods
- 7. H.H. Bauer, G.D. Christian and J.E. O'Reilly: Instrumental Analysis
- 8. J.W. Robinson, E.M.S. Frame and G.M. Frame II: Undergraduate Instrumental Analysis (7th Ed.)
- 9. R.D. Braun: Introduction to Instrumental Analysis

Course: Chem 535F Homogeneous and Heterogeneous Catalysis Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

The course is designed to introduce the homogenous and heterogeneous catalysis, reaction mechanism involving square planar and octahedral complexes. The students will learn to explain the mechanistic aspects of organometallic compounds and their relevance to chemical catalysis leading to hydrogenation, polymerization and catalytic reactions involving CO, NO, HCN and alcohols.

- 1. **Introduction (5 Lectures):** Definition and thermodynamics of catalysis, comparison between homogeneous and heterogeneous catalysis and their industrial applications.
- 2. **Inorganic Reaction Mechanism (15 Lectures):** Review of rate laws, activation parameters, substitution reaction on square planar and octahedral complexes, one electron and two electron transfer reactions. Inner sphere and outer sphere mechanism.

3. Addition Reaction (10 Lectures):

- (i) Hydrogenation, hydrobromination, hydrogenation of alkenes, alkynes and conjugated alkenes (Markovnikov and anti-Markovnikov products showing the intermediate stages), hydrogenolysis reaction to RhCl(PPh₃)₃ and RuCl₂(PPh₃)₃.
- (ii) Insertion reaction: Intramolecular and intermolecular insertion reactions and carbonylation of metal hydrides and metal alkyls.
- 4. **Transition Metal Hydrides (10 Lectures):** Synthesis, characterization, chemical behaviour of hydrido complexes, monohydride and dihydride catalysts, mono-, di-, tri- and polynuclear metal hydrides. Comparison the M–H and C–H groups by ¹H-NMR.
- 5. Wilkinson's and Related Catalysts in Hydrogenation (10 Lectures): Preparation of RhCl(PPh₃)₃, RhCl(CO)(PPh₃)₂, RuCl₂(PPh₃)₃, *cis-* and *tran*-RuCl₂(CO)₂(PPh₃)₂. Mechanism of hydrogenation of alkenes through oxidative and reductive elimination by rhodium(I) catalyst, RhCl(PPh₃)₃, RhH(PPh₃)₃.

6. Catalytic Reaction Involving CO and H₂ (20 Lectures):

(i) Hydroformylation reactions: cobalt catalysts, rhodium catalysts (Markovnikov and anti-Markovnikov) and other oxo catalysts.

- (ii) Fischer-Tropsch reaction and mechanism: Hydrogeneous Fischer-Tropsch catalysts, hydrogeneous model reactions and homogeneous CO hydrogenation.
- (iii) Ziegler-Natta polymerization and its mechanism.

7. Catalytic Reaction Involving Alcohols and HCN (10 Lectures):

- (i) Reductive carbonylation of alcohol and other compounds.
- (ii) Cluster compound in catalysis.
- (iii) Oxalate ester, synthesis of dialkyl oxalate and their mechanism using Pd, CO and NO.

Recommended Books:

- 1. Parcell and Kotz: Inorganic Chemistry
- 2. Cotton and Wilkinson: Advanced Inorganic Chemistry, 6th Edn. (1980)
- 3. J.P. Collman and L.S. Hegedus: Principles and Applications of Organotransition Metal Chemistry
- 4. J.E. Huheey: Inorganic Chemistry Principles of Structure and Reactivity
- 5. J.D. Atwood: Inorganic and Organometallic Reaction Mechanism
- 6. W.U. Malik G.D. Tuli and R.D. Madan: Selected Topics in Inorganic Chemistry
- 7. S.Z. Haider: Selected Topics in Inorganic Chemistry

Course: Chem 536F Environmental Chemistry Full marks: 100 (1.0 unit, 4 credits) Final examination: 80 marks, 4 hours Class assessment: 15 marks; Attendance: 5 marks

Intended Learning Outcomes (ILO)

The objectives of this course are to provide the knowledge of spheres of environment, natural cycles of environment, structure and compositions of hydrosphere and lithosphere. The course also provides the brief ideas about heavy metal pollution, sources, classification and disposal of wastes and hazardous substances, sources and characteristics of pollutants from some typical industrial effluents and their treatment.

1. **Introduction** (12 Lectures): Environmental chemistry, biogeochemical cycles, pollutants and contaminants, effects of pollutants on the biosphere:

biodegradability, toxicity and risks; minimization and prevention of pollution: Green Chemistry.

- 2. **Hydrosphere** (14 Lectures): Hydrological cycle; chemical composition of natural and sea water, carbon dioxide in water, dissolved oxygen in water, pH and alkalinity of natural water, behaviour of metal ions in water, complexing agents and humic substances in natural water, microbially mediated redox reactions, water quality parameters and standards, eutrophication, toxic metals in hydrosphere.
- 3. Lithosphere (14 Lectures): Composition of lithosphere, origin and development of soils, soil structure and classification, water and air in soil, inorganic, organic and biological components in soil, pH and buffering capacity of soils, acid-base and ion-exchange reactions in soil, micro- and macronutrients, heavy metals in soil.
- 4. **Heavy Metal Pollution** (14 Lectures): Essential and toxic heavy metals; pollution sources, toxicity, biochemical and toxicological effects of lead, mercury, cadmium, arsenic, chromium, selenium and radon, mechanism of arsenic contamination in ground water, mitigation of arsenic pollution.
- 5. Wastes and Hazardous Substances (12 Lectures): Introduction, sources and classification of hazardous substances and wastes, hazardous wastes in the geosphere, hydrosphere, atmosphere and biosphere, impact of hazardous wastes on human health, disposal methods of hazardous wastes.
- 6. **Pollutant from Industrial Effluents** (14 Lectures): Sources and characteristics of pollutants, waste water treatment techniques, treatment of some typical industrial effluents: textile, pulp and paper, fertilizers, leather tanning, sugar, electroplating, soap and detergent industries.

- 1. S.E. Manahan: Environmental Chemistry (6th Edn.)
- 2. A.K. De: Environmental Chemistry (5th Edn.)
- 3. S.S. Dara: A Text Book of Environmental Chemistry and Pollution Control
- 4. Colin Baird: Environmental Chemistry

- 5. Roy M Harrison: Principles of Environmental Chemistry
- 6. Ian L. Pepper, Charles P. Gerba and Mark L. Brusseau: Environmental and Pollution Science
- 7. Jorge G. Ibanez, Margarita Hemandez-Esparza, Carmen Doria-Serrano, and Arturo Fregoso-Infante: Environmental Chemistry: Fundamentals
- 8. B.K. Sharma: Environmental Chemistry (11th Edn.)

Course: Chem 531L Inorganic Chemistry Practical and Project Examination: 24 hours (4 days) Full Marks: 200 (2 units, 8 credits)

(i) Experiment and Project: 140 ; (ii) Continuous Class Evaluation: 60

Intended Learning Outcomes (ILO)

At the end of the course, the students will learn to prepare the transition metal complexes and characterize the synthesized complexes by measuring some physical properties and spectroscopic methods. They will also learn to apply the chemical and physical methods to separate and estimate some metal ions and anions.

Experiments in Inorganic Chemistry

- Preparation of 1,10-phenanthroline, ethylenediamine, orthophenyline diamine, picolinic acid, salicylic acid, oxalic acid, orthoamino benzoic acid complexes of Co(III), Cu(II), Ni(II), Cr(III), Fe(II), Fe(III); characterization by elemental, magnetic measurement and spectroscopic method.
- 2. Ion-exchange separation and estimation of some metal ions: Cu(II), Ni(II) Co(III) and some heavy metals.
- 3. Extraction and estimation of magnesium from green leaves
- 4. Estimation of arsenic in water.
- 5. Preparation of metal-acetylacetonate complexes and separation of metal complexes by chromatographic techniques.
- 6. Solvent extraction method: Separation and estimation of metal ions.

- 7. Preparation and characterization of thiocynate complexes of transition metals containing some monodentate and bidentate ligands.
- 8. Separation and estimation of metals from some inorganic drugs.
- 9. Synthesis and characterization of molybdenum oxide clusters.
- 10. Colorimetric determination of minute amount of cobalt, nickel, iron and magnesium.
- 11. Determination of chloride (Cl⁻) and nitrate (NO₃⁻) by colorimetric method

Recommended Books:

- 1. J. Bassett and others: Vogel's Textbook of Quantitative Inorganic Analysis
- 2. Skoog and West: Fundamentals of Analytical Chemistry
- 3. Schwarzenbach and Flaschka: Complexometric Titrations.

Course: Chem 599

Thesis on Inorganic/Analytical/Environmental Chemistry Full Marks: 200 (2 units, 8 credits)

- (i) Thesis: 150 marks
- (ii) Viva-voce on thesis: 50 marks

Marks Distribution for Class Attendance

The marks for attendance shall be distributed on the basis of following table:

Attendance	Marks	Attendance	Marks	Attendance	Marks
95-100%	20%	90-<95%	18%	85-<90%	16%
80-<85%	14%	75-<80%	12%	70-<75%	10%
65-<70%	8%	60-<65%	6%	<60%	00%

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