West Bengal State University
Barasat, North 24-Parganas
(Effective from Academic session : 2016-2017)

Department of Chemistry

TWO YEAR FOUR SEMESTER M.Sc. (CHEMISTRY) PROGRAMME

Objective of the Programme

The purpose of the postgraduate programme in Chemistry at West Bengal State University is to provide knowledge base and laboratory resources to prepare students for careers as professionals in the field of chemistry, for doctoral research in chemistry, spectroscopy, biological chemistry and related fields, and to prepare the students with a chemistry background that will allow them to become effective scientist or teachers in higher education.

● To provide the students with a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Inorganic & Analytical, Organic and Physical Chemistry.

● To enable the students to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.

● To impart to the students reasonably skills in problem solving, critical thinking and analytical reasoning with application to scientific problems.

● To prepare the students in such a manner so that they can clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.

● To aid the students in developing the ability to explore new areas of research in both chemistry and allied fields of science and technology.

● To make the students well prepared so that they will be able to function as a member of an interdisciplinary problem solving team.

COURSE STRUCTURE

Semester	I		II		III		IV		Total Marks
Marks	300		300		300		300		1200
Course Type	Theo	Pract	Theo	Pract	Theo	Pract	Theo	Lab	
General (G)	180	120	180	120	210	90	80	40[@]	1020
Elective (E)							100	80*	180
Total Marks	180	120	180	120	210	90	180	120	1200

Elective Courses (E) in Different Branches of Chemistry: Physical/Inorganic/Organic

[@] Laboratory Related Assignment
* Project work and Literature review

Semester	I	II	III	IV	Total
Credit Points	24	24	26	26	100

SEMESTER I

Marks 300
Total Credit Points (CP) : 24

Paper	Course ID	Course Taught	Marks		Total Marks
	CHEM		Theo	Pract	
I (Inorganic)	217111	• Symmetry and bonding • Coordination Chemistry-1 • Meta- ligand equilibrium in solution • Biioinorganic Chemistry-1 • Electrochemical Analysis	60	40	100 (CP = 8)
II (Organic)	217112	• Structure Activity Relationship • Stereochemistery • Pericyclic Reaction • Organic Reaction Mechanism • Natural Products-Terpenoids	60	40	100 (CP = 8)
III (Physical)	217113	• Introductory Quantum Mechanics • Symmetry and Group Theory • Kinetics • Thermodynamics • Fundamentals of Spectroscopy	60	40	100 (CP = 8)
			180	120	300 (CP = 24)

SEMESTER II

Marks 300

Total Credit Points (CP) : 24

Paper	Course ID	Course Taught	Marks		Total Marks
	CHEM		Theo	Pract	
IV (Inorganic)	217121	• Coordination Chemistry-2 • Organometallics-1 • Solid State • Chemistry of Elements-1 • Bioinorganic Chemistry-2	60	40	100 (CP = 8)
V (Organic)	217122	• Synthetic Methodology • Synthetic Strategy • Asymmetric Synthesis • Natural Products and Steroids • Bioorganic Chemistry	60	40	100 (CP = 8)
VI (Physical)	217123	• Quantum Mechanics-2 • Statistical Mechanics-1 • Macromolecules • Electrochemistry-1 • Biophysical Chemistry	60	40	100 (CP = 8)
			180	120	300 (CP = 24)

SEMESTER III

Marks 340

Total Credit Points (CP) : 26

Paper	Course ID	Course Taught	Marks		Total Marks
	CHEM		Theo	Pract	
VII (Spectroscopy)	217211	• NMR Spectroscopy, Theory and Application • Mossbauer and Photoelectron Spectroscopy • Emission Spectroscopy • EPR Spectroscopy • Mass and IR	60	-	60 (CP =5)

		Spectroscopy			
VIII (Inorganic)	217212	• Crystallography • Nuclear Chemistry and Radiochemical Analysis • Organometallics-2 • Chemistry of Elemnts-2	50	30	80 (CP = 7)
IX (Organic)	217213	• Organometallics • Photochemistry • Carbohydrates, Nucleotide and Nucleoside • Supra-molecular Chemistry	50	30	80 (CP = 7)
X (Physical)	217214	• Quantum Mechanics-3 • Statistical Mechanics-2 • Nanomaterials • Electrochemistry-2	50	30	80 (CP = 7)
			210	90	300 (CP = 26)

SEMESTER IV

Marks 260

Total Credit Points (CP) : 22

Paper	Course ID	Course Taught	Marks		Total Marks
	CHEM		Theo	Lab	
XI (General)	217221	• Inorganic Rings, Cages and Clusters • Inorganic Reaction Mechanism • Reagents in Organic Synthesis • Green Chemistry • Laser • Theoretical Spectroscopy	80	20[@]	100 (CP = 9)
XII (Elective)	217222	Inorganic: • Group Theory • Magnetochemistry • Advance Bioinorganic Chemistry -3 • Spectroscopic Analysis of Inorganic Compounds Organic: • Stereochemistry and Advance Pericyclic Chemistry • Medicinal Chemistry • Heterocycles • NMR Spectroscopy Physical: • Advance Quantum	80	20[*]	100 (CP = 9)

		Mechanics • Statistical Mechanics-3 • Non equilibrium Thermodynamics • Advance Photophysics • Modern Material Chemistry		
XIII (Project)	217223		$20^{\#}$ $80^{\$}$	100 (CP = 8)
			180 120	300 (CP = 26)

[@] Laboratory Quiz

*** Grand Viva**

 # Literature Review and report submission on a specific topic

$ Project work and Computer Lab

Semester I

Inorganic Chemistry (Paper I)

Course specific objective :

This course is designed to introduce the students to the basic inorganic chemistry of PG level. The concepts that were dealt with qualitative approach like VB theory and MO theory will be established by theoretical calculations. Moreover properties of metal complexes in solid state and in solution state will be discussed here. Basic bioinorganic chemistry will give the students the concept of different in vivo processes and role of metalloenzymes. Students will also get an idea about the evaluation of redox properties of metal complexes in solution by different advanced methods like CV, polarography etc.

Unit-1. Symmetry and Bonding 12M

Symmetry in nature, symmetry elements and symmetry operations. Symmetry properties of atomic orbitals. Elements of group theory, multiplication tables, point groups and their stereographic projections.
Born-Oppenheimer approximation, LCAO-MO and VB treatments on H_2^+, H_2 ; application to homo- and hetero- nuclear diatomic molecules/ ions of second period elements, electron density, forces and their role in chemical bonding. Hybridization and valences, MO's of H_2O, NH_3, CH_4; Huckel – pi – electron theory and its applications to ethylene, butadiene and benzene, idea of self consistent field. Concept of resonance.

Unit 2 : Co-ordination Chemistry 1 12M

Crystal filed theory, Splitting of d-orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyrimidal, square pyramidal and octahedral fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environment, hole formalism, inversion and equivalence reactions, splitting of d^n terms in octahedral and tetrahedral fields, Octahedral site preference energy, Tetrahedral distortion and Jahn Teller effect. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of

complexes (Irving Williams order). Kinetic aspects of crystal field stabilization. Crystal field activation energy. Labile and inert complexes, Limits of applicability of crystal field theory. Shapes of complexes.

Unit 3 : Metal ligand equilibrium in solution **12M**

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic effect. Spectrophotometric and pH metric determination of binary formation constants.

Unit 4 : Bio-inorganic chemistry 1 **12M**

Elements of life, Essential and trace elements in biological systems. Basic reactions in the biological systems and roles of metal ions in biological processes. Bioenergetic principle and role of ATP. Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Transport across biological membrane – Na^+-K^+-ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, urease. Metal dependent diseases: Wilson's disease, Alzheimer disease. Metal complexes as drugs: Pt, Rh, Ru and Au drugs. Toxic effects of metal ions, detoxification by chelation therapy.

Unit 5 : Electrochemical analyses **12M**

Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry

Practical: **40M**

Course specific objective :

Practical is so designed to introduce the students to synthetic methodologies for the preparation of different coordination complexes. This hand on experiments will also help them to be skilful in dealing with various chemicals, purification, crystallisation etc. Students will be introduced to different quantitative analysis also including spectrophotometric estimation of single metal ion. This hands on training will help the students to handle the spectrophotometer and they will get the confidence to use the instruments for more detail analysis in the subsequent semesters.

(A) Synthesis of some metal complexes: tris(ethylenediamine)nickel(II) thiosulphate, tris(acetylacetonato)manganese(II), hexaminecobalt(III) chloride, mercury tetrathiocyanatocobaltate(II), Reineki salt, bis(biguanido) copper(II) sulphate

(B) Complexometric Estimation of Fe(III) and Al(III) mixture, Cu(II) and Zn(II) mixture

(C) Spectrophotometric Determination of i) Fe(II) in mixture, ii) Mn(II) in mixture

Organic Chemistry (Paper II)

Course specific objective :

To introduce the students to the basic theoretical excellence and calculations that are involved in assuming and proving various organic molecular properties *viz.* aromaticity, acidity-basicity, reactivity, rate of reactions *etc*. This course is also designed on the one hand to impart the PG-students a thorough knowledge about themechanisms of reactions of some specific category of important organic reactions whereas on the other hand they will have basic knowledge of some natural products too. The students would also be introduced to higher level of learning of stereo chemical phenomena, their application towards the understanding to pericyclic and other reactions of organic molecules.

Unit 1 : Structure Activity Relationship **12M**

MO treatment of acyclic and cyclic conjugated systems. Huckel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes (C_{60}), alternate and non alternate hydrocarbons, anti aromaticity, pseudoaromaticity, homo-aromaticity. Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene systems.

Unit 2 : Stereochemistry **12M**

Acyclic systems upto 4 chiral centers. Compounds with asymmetric carbons in branched chains, symmetry, point groups. Correlation of axial dissymmetry and centrodissymmetry. Nomenclature of compounds involving axial and planar chirality. Winstein-Holness equation. Curtin Hammett principle. Conformational analysis of cyclohexane, cyclohexene, decalins and their derivatives. Effect of conformation on reactivity in acyclic compounds and cyclohexanes.

Unit 3 : Pericyclic Reactions **12M**

Classification and stereochemical modes. Thermal and photopericyclic reactions. Selection rules and stereochemistry of electrocyclic reactions. 2-component cycloadditions. Sigmatropic rearrangement. Carbene addition. Rationalization based on Frontier MO approach, correlation diagrams. Dewer-Zimmermann approach. Mobius and Huckel systems. Sommelet, Hauser, Cope and Claisen rearrangements. Ene reactions, Wittig rearrangement.

Unit 4 : Organic Reaction Mechanisms **12M**

Reactive intermediates – Formation and stability of classical and non classical carbonium ions, carbanions, carbenes, nitrenes, radicals and arynes. Nucleophilic. Electrophilic and radical substitution, addition and elimination reactions. Methods of determining reaction mechanisms. Kinetic isotope effect. Hard and soft acids and bases. Hammett equation.

Unit 5 : Natural Products – Terpenoids **12M**

Isoprene rule. Structure elucidation (by chemical and spectroscopical methods). Synthesis, Biogenesis and Biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. Structural types, General introduction to sesqui-, di- and tri- terpenoids.

Practical **40M**

Course specific objective :

Practical is so designed to introduce the students to some organic synthetic methodologiesinvolving 'Green' approach. This hand on experiments will also help them to be skilful in dealing with various chemicals, purification, crystallisation using different kind of solvents during the practical classes of organic molecules and the concept of greenness of a chemical reaction will also be familiar to them.

Synthesis of some organic compounds (involving some Green methodologies also) and their Spectral analysis.

Physical Chemistry (Paper III)

Course Specific Objective:

- To make the students learn the fundamentals of quantum chemistry and its applications to simple systems
- To make the students learn the basic concepts and applications of group theory,
- To learn the theoretical background for the different theories in chemical kinetics
- To extend the knowledge in thermodynamics learned in the UG course in different application areas
- To expose the students to slightly higher level about the basic concepts of spectroscopy

Unit 1 : Introductory Quantum Mechanics **12M**

Postulates of quantum mechanics and their analysis; Properties of operators and commutators; Hermitian operators and their properties; Time-independent Schrodinger equation; Concept of stationary states, Free particle, Particle in a ring, Barrier problems and tunneling phenomenon ; Equation of motion; Ehrenfest's theorems, Angular momentum operators, Eigenvalues and eigenfunctions, Hydrogen atom, Spherical Harmonics

Unit 2 : Symmetry & Group Theory **12M**

Symmetry elements and operations; Classification of molecules; Group, subgroup etc., class, character; point groups, point group symbols; representations; great orthogonality theorem and its consequences; character table. Symmetry adapted linear combination (SALC) with illustrative examples.

Unit 3 : Kinetics **12M**

Collision theory and activated complex theory. Ionic reactions, kinetic salt effects. Steady state kinetics, kinetic and thermodynamic control of reactions. Unimolecular reactions. Chain reactions. Photochemical and oscillatory reactions. Autocatalysis.

Unit 4 : Thermodynamics **12M**

Brief resume of the concept of free energy, entropy and laws of Thermodynamics and general condition of Equilibria. State functions. Legendre transformation. Dependence of thermodynamic functions of composition: partial molar quantities, their significance and methods of determination. Thermodynamics of ideal and non-ideal binary solutions, excess function for non-ideal solutions and their determination.

Unit 5 : Fundamentals of spectroscopy **12M**

General introduction, nature of electromagnetic interaction, shapes and width of spectral lines, intensity of spectral lines, Fourier transform, Microwave spectroscopy : Moment of inertia and classification of molecules, Energy expression for symmetric rotor, Non rigid rotator, Vibrational-Rotational spectra of diatomic molecules, Breakdown of the Born-Oppenheimer approximation : The interaction of Rotation and Vibration.

Practical **40M**

Course Specific Objective :

● To learn the use of basic equipments spectrophotometer, potentiometer, pH-meter, polarimeter and conductivity meter.

● To learn to carry out various spectrophotometric, potentiometric and conductometric titrations

One day based physicochemical experiments.

1. pH-metric titration of a polybasic acid and determination of its basicity and dissociation constants

2. Determination of Solubility product of lead (II) iodide

3. Conductometric titration of a mixture of halides ($KCl+HCl+NH_4Cl$) by (i) NaOH and (ii) $AgNO_3$

4. Spectrophotometric determination of pK_{in} of Bromocresol Green and determination of isosbestic point

5. Potentiometric titration of (KI+KCl) mixture by silver nitrate

6. Determination of E^0 of the Quinhydrone electrode by potentiometric method

7. Determination of hydrolysis constant of a salt by a pH-meter

8. Spectrophotometric study of the alkaline hydrolysis of crystal violet. Determination of rate constant and order with respect to alkali

Semester II

Inorganic Chemistry (Paper IV)

Course specific objective :

In this course the students will learn some advanced topic like crystal filed theory and bioinorganic chemistry as a continuation of the earlier semester. The course of organometalic chemistry will be introduced here. This portion will enable them to understand different kinds of bonding including η bonding. Solid state chemistry course will give an idea about band theory and introduce them to the field of superconductor

Unit 1: Coordination Chemistry 2 **12 M**

Electronic spectra of transition metal complexes : Microstates, determination of ground and excited state terms of d^n ions; Orgel diagrams (qualitative approach), selection rules for spectral transitions, *d-d* spectra of d^n ions and crystal field parameters, nephelauxetic series. Metal-ligand bonding (pictorial MO approach): sigma and pi-bonding in complexes, CT transitions.
Crystal field splitting of free ion terms in weak and strong crystal fields (Oh and Td), energy level diagrams and symmetries and multiplicities of energy levels in strong crystal fields,
Construction of mo diagrams of polyatomic molecules including coordination complexes (Oh and Td), sandwich complexes: (ferrocene, dibenzenechromium).

Unit 2: Organometallics 1 **12 M**

Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with examples
Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and cyclopentadienyl complexes. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$ and $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit 3: Solid state **12 M**

Crystal defects and Non- Stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects- point, line and plane defects, vacancies- Schottky and Frenkel defects. Determination of equilibrium concentrations of Schottky and Frenkel defect formation, non-stoichiometric defects, colour centres in ionic crystals, stoichiometric imbalance in crystals**.**
Bonding in metal crystals: Free electron theory of metals, specific heat, Hall effect and its quantum manifestation, Band theory of metals: band gap, electrical and thermal conductivity of metals, p-n junction semi-conductors (intrinsic and extrinsic), insulators, rectifiers and transistors, super conductors.

Unit 4: Chemistry of Elements 1 (Special Features) **12 M**

d-Block Elements

Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr- Hf , V-Nb-Ta, Cr- Mo- W, Mn-Tc-Re and Pt group metals.

Mixed valence compounds of Fe, Cu, Pt; Fe-S compounds, cobaloxime related compounds, conformational changes and thermochromism of Ni(II) compounds, Ru(II) and Ru(III) compounds, oxo compounds of Ru and Os, Rh(I) and Ir(I) carbonyl halide and carbonylhydrides. Aqueous chemistry of Be^{II} and Al^{III}, basic beryllium compounds.

Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo-blue, W-blue, Pt-blue, W-bronze, Ru-red.

Unit 5: Bioinorganic Chemistry 2 **12 M**

Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes.

Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (ferredoxines). Respiratory electron transport chain, cytochrome c oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems, model study.

Practical **40M**

Course specific objective :

The practical classes are designed to impart the knowledge to the students by both qualitative and quantitative experiments. Students will be familiar with the different processes by which the metal ions can be determined in solution in presence of other metal ions. Composition of metal complexes will be determined by quantitative analysis. Students' interpreting skill, logical method of analysis would be augmented by means these study.

(1) Semi-Micro Qualitative Inorganic Analysis:

Semi-Micro Qualitative Inorganic Analysis of complex inorganic mixtures containing not more than six (6) inorganic radicals from the lists **(a), (b), (c),** and **(d),**of which two (2) radicals must be derived from the rare elements **(d)**, and the mixture should not contain more than one insoluble material from the lists **(c),** and **(d),** :

(a) Cation Radicals derived from:
Ag, Hg, Pb, Bi, Cd, Cu, As, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, Na, K and NH_4^+ ion.

(b) Anion Radicals:
F^-, Cl^-, Br^-, I^-, BrO_3^-, IO_3^-, SCN^-, S^{2-}, $S_2O_3^{2-}$,SO_3^{2-}, SO_4^{2-}, NO_2^-, NO_3^-, PO_4^{3-}, AsO_3^{3-}, AsO_4^{3-}, BO_3^{3-}, H_3BO_3, SiO^{2-}, CrO_4^{2-}, $Cr_2O_7^{2-}$, $[Fe(CN)_6^{4-}]$, $[Fe(CN)_6^{3-}]$.

(c) Insoluble Materials:
$PbSO_4$, $BaSO_4$, $SrSO_4$, $PbCrO_4$, CaF_2, SiO_2 and various silicates, SnO_2, Al_2O_3, Fe_2O_3, Cr_2O_3, AgCl, AgBr, AgI.

(d) Cation radicals, anion radicals and insoluble materials derived from the following rare Elements: V, Mo, W, U, Ti, Zr, Ce, Th and Be.

(2) Advanced Physicochemical Experiments

Model Experiments

1.Determination of composition of complexes formed in solution by spectrophotometric methods:
(a). Mole-ratio method
(b). Slope- ratio method
(c). Job's method of continuous variation

Model systems:
(i). Fe^{III}-sulfoslicylic acid complex
(ii). Fe^{II}- (1,10- phenanthroline) complex
(iii). Cu^{II}- ethylenediamine complex
(iv). Zn^{II}-alizarin-S complex

2. Determination of stability constants of metal-ligand complexes by pH-metric methods:
Model systems:
(i). Cu^{II}- glycinate complexes
(ii). Cu^{II}-sulfosalicylate

Organic Chemistry (Paper V)

Course specific objective :

The basic concepts of designing an organic molecule synthesis is introduced here. This idea will automatically relate to the knowledge of using specific reagents and the knowledge of reaction conditions for synthesis in particular. Accordingly, some advanced level of information of organo-main group reagents and asymmetric synthesis are introduced here. Keeping this orientation in mind the students will be introduced to some naturally occurring macromolecules, their structural features and the challenges towards their synthesis.

Unit-1: Synthetic Methodology 12M

Organoboron: Chemistry of organoboron compounds; Carboranes; Hydroborations; Reduction; Reactions of organoboranes; Unsaturated hydrocarbon synthesis; Allyl borane and boron enolates.

Organophosphorus: Chemistry of organophosphorus compounds; Phophorus ylides; Wittig reaction and its modofications; Chiral phosphines; Phosphine-oxides and its applications.

Organosulphur: Chemistry of organophosulphur compounds, Sulphur stabilization of anions and cations, Sulphonium salts, Sulphonium and sulphoxonium ylides, Chiral sulphoxides

Organosilicon: Chemistry of organosilicon compounds; Synthetic uses of silyl ethers; Silyl enol ethers; TMSCl, TMSI, TMSCN, Alkene synthesis, Alkenyl, Vinyl, Aryl, Allyl and Acyl silanes; Brook rearrangement; Silicon Baeyer-Villiger rearrangement.

Unit-2: Synthetic Strategy **12M**

Retro-synthetic analysis; Disconnection approach; Typical examples to illustrate the disconnection approach; FGI; Umpolung(1,3-dithiane); Convergent synthesis; One-group, Two-group disconnections; Selectivity aspects: Chemo-, Regio-, Stereo -selectivity; Retron; Uses of aliphatic nitro and amines. Protection and deprotection of common functional groups (Hydroxy, Carbonyl, Carboxylic and Amino groups)

Unit-3: Asymmetric Synthesis **12M**

Principles and newer methods of asymmetric synthesis (Including enzymatic and catalytic nexus); Enantio and diastereo selective synthesis; Addition to carbonyl compounds; Reactions of enolates (α-substitution), Alkylation, Asymmetric aldol reaction, Addition to C-C double bond(Electrophile induced cyclization, iodolactonization, hydroboration,conjugate addition, Diels-Alder cycloaddition, cyclopropanation); Reduction of C-C double bond; Carbonyl and Imine groups; Oxidation, Epoxidation, Dihydroxylation, and mono-hydroxylation; Rearrangement: [3,3]-sigmatropic, [2,3]-Wittig,Alkene isomerisation, Hydrolysis and esterification.

Unit-4: Natural Products and Steroids **12M**

Familiarity with methods of structure elucidation (Chemical and spetroscopical methods);
Bio-synthesis; Synthesis and Biological activity of alkaloids (Nicotine, atropin)
General methods of study and structural types; Chemistry of cholesterol, hormones, bile-acids

Unit-5: Bioorganic Chemistry **12M**

Molecular models of biological receptors, Biomimetic chemistry, Design, Synthesis and binding studies of synthetic receptors, Enzyme models, Micelles, Cyclodextrins, Polymers, Remote functionalisation reaction, Catalytic antibodies, Principles of gene synthesis, Proteins, Peptides and Amino acid.

Practical **40M**

Course specific objective :

Practical classes are oriented in the direction to develop the students' hand on skills in separating organic compounds, the identification of some specific functional groups. They also will learn to specific chemical transformations needed for specific functional groups. Accordingly, thereto determine the nature of organic compounds and the organic compound in particular by means of derivatisation and by means of melting point determination also introduced to the students.

Identification of solids from mixture of two solids: Separation on the basis of solubility, Detection of functional group(s) present in each constituent organic compound, Identification

of two solids individually by means of checking melting point of the compounds and their corresponding derivatives with the help of the melting points reported in literature.

Physical Chemistry (Paper VI)

Course specific objective :

- To learn approximation theorems for applications to simple problems of interest
- To learn the basic concepts of statistical thermodynamics for calculation of various thermodynamic properties of molecular systems
- To learn in details about polymers
- To learn and understand the theories of electrochemistry
- To learn various aspects of bio-physical chemistry

Unit-1: Quantum Mechanics 2 **10M**

Rigid Rotator, Ladder operators ; Harmonic Oscillator, Calculation of various quantities (matrix elements, selection rule, etc) using ladder operators and recursion relations of Hermite polynomials, Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom)

Unit-2: Statistical Thermodynamics I **10M**

Entropy and Probability; Ensembles-Types; Partition Function and Thermodynamic properties; Maxwell Boltzmann distribution. The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases ; Calculation of thermodynamic properties of ideal gases in terms of partition function. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

Unit-3: Macromolecules **10M**

Definition of Polymers; Types of Polymers; Polymerization process – condensation, addition, radical chain, ionic, condensation polymerization, copolymerization; Kinetics of Polymerization, chain transfer, retardation, inhibition; Polymerization in homogeneous and heterogeneous systems; Polymerization conditions; Mechanisms of polymerization; Molecular mass of Polymers, their determination.

Unit 4 : Electrochemistry 1 **10M**

Debye Huckel theory and its extension. Debye Huckel Onsager theory and its extension. Ion solvent interactions. Electrode surfaces, potential and measurements, thermodynamics of such systems. Lippman equation. Gouy Chapman & Stern models.

Unit-5: Bio-physical Chemistry **20M**

Protein structure- primary, secondary, tertiary and quarternary structure; protein denaturation; Titration curves; Forces Involved in Biopolymer Interactions; Ligand binding to Bio-polymers; Bioenergetics; Ion Transport through Cell Membrane; Nerve Conduction, Muscular Contraction and Energy Generation in Mechanochemical System.

Practical **40M**

Course Specific Objective :

● To learn to apply conductometry for verification of Onsager equation, determination of acid dissociation constant and solubility product of a sparingly soluble salt and cmc of a surfactant.
● To learn to measure rate and order of a chemical reaction
● To learn to experimentally determine standard electrode potential of a redox couple
● To use viscometer for determination of isoelectric point of an amino acid

One/Two day based physicochemical experiments.

1. Verification of Onsager equation and determination of λ^0 and K_a of acetic acid

2. Verification of the Onsager equation and conductometric determination of solubility product of a sparingly soluble salt

3. Determination of critical micelle concentration of SDS by conductometry

4. Determination of the standard redox potential (E^0) of ferrocyanide-ferricyanide system.

5. Kinetic study of the iodination of aniline by colorimetric method

6. Determination of isoelectric point of gelatine

7. Kinetic study of the reaction between $K_2S_2O_8$ and KI and study on the effect of added salt on the rate constant.

8. Study of the determination of the decomposition of hydrogen peroxide by acidified KI, maintaining a constant excess of iodide. Determination of the rate constant at four different temperatures and hence determination of the energy of activation, enthalpy of activation and entropy of activation of the reaction.

Semester III

Spectroscopy (Paper VII)

Course Specific Objective :

Spectroscopy is an essential tool for the identification and analysis of chemical compounds. In this course the students will be exposed to the different areas of the electromagnetic spectrum which shows the spectra corresponding to the different vibrations, relaxations and transitions in a chemical compound. The basic theoretical alongwith application and analysis of the different types of spectroscopy will be taught to the students. The course should give the student enough idea as to interpret when a spectra of an unknown compound is given to him.

Unit-1 : Nuclear magnetic resonance spectroscopy – theory & applications 12M

Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical sift, deshielding, spin-spin interactions, factors influencing coupling constant `J`. Classification of molecules: (ABX, AMX, ABC, A_2B_2, etc. types), spin decoupling. FT-NMR (qualitative idea) and its advantages, Introduction to CMR: Basic idea. Sesitivity, Proton decoupled and non-decoupled CMR, Off Resonance CMR, Applications of NMR in medical diagnosis.

Unit-2 : Mossbauer spectroscopy 12M

Principle, experiment, line-width center shift, quadrupole interaction, magnetic interaction, information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in varieties of environments

Photoelectron spectroscopy
Photo excitation and photoionization, core level photo ionization (XPS, ESCA.) and valence level (UPS) experiments, detection of atoms in molecules, chemical shift, differentiating same element in different environments.

Unit-3 : Emission spectroscopy 12M

Franck-Condon principle, Mirror-image symmetry and its violation, Radiative and radiationless deactivation, Oscillator strength, Polarization characteristics of emission, Quenchers and life-time variations

Unit-4: Electron spin resonance spectroscopy 12M

Basic principles, zero field splitting, and Kramer`s degeneracy, factors affecting the `g` value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship. Basic instrumentation, measurement techniques and simple applications.

Unit-5 : Mass & IR spectroscopy **12M**

Mass spectroscopy
Basic instrumentation, ion production - EI,CI, FD and FAB techniques, Mass spectral fragmentation of typical organic compounds, common functional groups.

IR spectroscopy
Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance, FT IR.

Inorganic Chemistry (Paper VIII)

Course Specific Objective : This course will help the PG-students towards the understanding of advanced level of organometallic chemistry including some catalytic cycles. This portion will give them an idea about the industrial methods of preparation of alkenes and alkynes by oligomerization and metathesis reactions. Introduction to crystallography will give them an idea for determining the structure by various methods. Different radiochemical methods and nuclear model study will enable to have a detailed idea about the core structure of an atom. As a continuation of group chemistry, a portion of lanthanides and actinides portion will be here so that students become familiar with elements having similar property.

Unit 1: Crystallography **14M**

Fundamentals of X-ray crystallography, crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their properties, Diffraction of x-ray, lattice planes, indices, Brag's condition, reciprocal lattice, Brag's law in reciprocal, Geometric data collection (simple examples), structure factor, systematic absence, heavy atom method. Fourier synthesis, Patterson function, experimental diffraction methods (Laue method, rotating crystal method).

Unit 2: Nuclear Chemistry & Radiochemical Analysis **12 M**

Nuclear models: Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism.
Nuclear reactions: Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.
Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

Unit 3: Organometallics 2 **12M**

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.
Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples.
Catalysis by Organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkens and alkynes, Zieglar- Natta catalysis , photo dehydrogenation catalyst (platinum POP).

Unit 4: Chemistry of elements 2 **12M**

f– Block Elements: Lanthanide and Actinide Elements:
Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry; electronic spectra and magnetic properties. Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples).
Compounds of Sc, Y, La and Ac; Ce(III) and Ce(IV) compounds and their reactions, Lanthanide compounds as high temperature superconductor, nmr shift reagent and MRI reagent.

Practical **30M**

Course Specific Objective :

The practical classes are designed to impart the knowledge to the students regarding Quantitative analysis of complex materials, such as, ores and alloys. This portion is totally relevant to industry as the methods are industrial methods. This will give the students an opportunity to get acquainted with hands on training on different methods. The students will handle the instruments like UV, IR *etc.* on their own and also interpret data so skills to handle modern instruments will be developed.

(1) Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and/or instrumental methods as applicable.

Model Samples

Ores, Minerals , Concentrates:

Dolomite ($CaCO_3$, Mg CO_3, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys:

Brass (Cu, Zn); Soldier / Type metal (Pb, Sb, Sn); Bronze(Cu, Zn, Sn), Aluminium bronze(Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P).

Mixture:
Chromium (III) and Mn(II) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the lab. session.

(2) Kinetics studies on redox reactions:

(A) Model system:
Determination of the rate constants of reduction of the complex, $[Co(NH_3)_5 (N_3)]Cl_2$, by aqueous Fe^{2+} ions by spectrophotometric method.

Kinetics studies on linkage isomerism:

(B) Model system:
Kinetic investigation of transformation of the complex,
$[Co(NH_3)_5 (ONO)]Cl_2$ to $[Co(NH_3)_5 (NO_2)]Cl_2$ by spectrophotometric method.

Kinetics studies on substitution reactions:

(C)Model system:
Kinetic investigation of the substitution reaction,
$[Co(NH_3)_5 (SO_3)^+] + NO_2^- \rightarrow$ by spectrophotometric method.

(D) Kinetics studies on protolysis reaction:

Model system:
Kinetic investigation on protolysis of the complex, $[Co(NH_3)_5 (CO_3)^+]$ ion by spectropotometric method.

(3) **Spectroscopic Studies on Model Compounds**

Analysis of supplied UV-VIS, IR, magnetic moment data and cyclic voltammogram of model compounds.

Organic Chemistry (Paper IX)

Course Specific Objective :

This course would enable the students to get the knowledge of some spectroscopic techniques and their application to interpret the structural features of molecules. The deliverable knowledge to the students based on how these spectroscopic techniques could be used to judge the purity, architectural features, and properties of compounds is the key idea of this course. On the other hand the Pg-students also learn the host-guest chemistry that is being continuously used in biological systems and also by the synthetic chemists. Introduction to photochemical transformations and some relevant naturally occurring macromolecules to the students have been made here too.

Unit-1: Organometallics **14M**

Synthesis, Structure, Bonding, Oxidative insertion, Reductive elimination, Ligand migration from metal to carbon, Organometallic reagents in organic synthesis and in homogeneous catalytic reactions (Hydrogenation, Hydroformylation, Isomerisation and Polymerisation), Pi-acid metal complexes, Activation of small molecules by coordination,
Coupling reaction: Heck reaction, Stille, Suzuki, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, Functional organometallic compounds, Use of Indium and Zinc.

Unit-2: Photochemistry **12M**

Basic principles, Jablonski diagram, Direct and sensitized reactions, Photochemistry of olefinic compounds; cis-trans isomerisation; Patterno-Buchi reaction; Norish type-I and Norish type-II reaction; Photo-reduction of ketone; Di-pi methane rearrangement; Photochemistry of arynes; Photo-reaction in solid state; Radical initiators; Reactivity pattern of radicals; Substitution and addition reactions involving radicals; Cyclisation of radicals.

Unit-3: **12M**

Carbohydrates

Basic structure and type of sugars; Protection and deprotection, Deoxysugars, aminosugars, glycalsugars and their synthetic aspects, Synthetic approach (Combinatorial) towards polysachharides of biological and industrial importance, Carbohydrate as chiral pools in organic synthesis.

Nucleoside and Nucleotide

Chemical synthesis of nucleosides and oligonuleotides, Bio-synthesis of nucleotides and folic acids, Replication, transcription- Protein bio-synthesis, Covalent interaction of nucleic acids with small molecules, Structural features of DNA and RNA.

Unit-4: Supramolecular Chemistry **12M**

From molecular to supramolecular chemistry: Factors leading to strong binding (non-covalent interation), New molecular receptors, Crown ether, Sidero force, Cyclophanes, Cyclodextrin and their application in specific recognition processes., Supramolecular reactivity and catalysis, Switching devices, self assembling, self replication of supramolecular aggregates and auto-catalysis.

Practical **30M**

Course Specific Objective :

The practical classes are designed to impart the knowledge to the students regarding isolation and purification of some common naturally occurring macromolecules. The students also will learn to synthesise some targeted molecules, organic reagents and to purify them using column chromatography. Students' interpreting skill, logical method of analysis would be augmented by means of confirming these isolated and synthetic compounds by spectroscopic data. The students will handle the instruments like UV, IR *etc.* on their own thus skills to handle modern instruments will be developed.

Extraction and purification of some natural products.
Synthesis of some useful reagents and their uses in synthesis.

Physical Chemistry (Paper X)

Course Specific Objective :

- To learn quantum mechanical treatment of theories of valence and chemical bonding
- To learn the development and application of quantum statistics
- To learn about nanomaterials and electrode kinetics

Unit-1 : Quantum Mechanics 3 **14M**

Ground and excited state of helium atom. Pauli's Exclusion principle. Many-electron atoms. Concept of spin and determinantal wavefunctions, Anti-symmetry principle and antisymetrization operator, Independent particle model, Theories of valence, Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments and their equivalence limit. Virial theorem and chemical bonding

Unit-2 : Statistical Mechanics 2 **12M**

Phase space and ergodic hypothesis, Gibbs paradox and Sackur-Tetrode equation, system of interacting molecules-imperfect gas, Quantum statistics, BE and FD statistics, Specific heat of electron gas, Bose condensation. Liouville theorem and its consequences, its quantum version. Formulation of Quantum statistics-density matrix.

Unit-3 : Nanomaterials **12M**

Nano-world-definitions and properties, typical synthetic strategies for nanomaterials, characterization and applications

Unit-4 : Electrochemistry 2 **12M**

Electrode kinetics-Nernst, Butler-Volmer equation, Tafel equation, Overpotential, corrosion, photoelectrochemical splitting of water

Practical **30M**

Course Specific Objective :

- To learn to study the kinetics of iodine clock reaction, autocatalytic reaction and inversion of sucrose

● To learn to determine the equilibrium constant of a reaction
● To learn to determine by potentiometry the equivalence point of titration of a weak acid by a strong base and standard electrode potential of a redox couple

One/Two day based physicochemical experiments

1. Studies on kinetics of iodination of acetone

2. Kinetic study of the autocatalytic reaction between potassium permanganate and oxalic acid

3. Determination of equilibrium constant of acid hydrolysis of an ester

4. Potentiometric titration of acetic acid by sodium hydroxide using quinhydrone electrode

5. Determination of E^0 of Ag/Ag^+ system. and activity coefficient of Ag^+ ions

6**.** Kinetic study of the inversion of sucrose

Semester IV

Paper XI (GENERAL)

Course Specific Objectives : This course would enable the students to get the knowledge of cluster compounds. Concept of different structural topologies will be discussed here along with their effectiveness as catalysts. Students will also be introduced to electron transfer processes in solution which will enable them to interpret electron transfer mechanism.

Unit-1 : **25M**

1A :Inorganic Rings, Cages and Clusters **12M**

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds-Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

1B: Inorganic Reaction Mechanism **13M**

Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.
Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Four broad classes of mechanism of substitution-D, A, Ia and Id. Mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms.

Unit-2 : 25M

Course specific objective:
Chemicals and Chemistry are basically intimate part of our day to day life and lifestyle. Starting from the food we consume related to agricultural industry, the drugs we need related to pharmaceutical industry or any single item we use related other sorts of industries for our lifestyle management are someway related to the world of chemicals and chemistry. Naturally, this portion of course is designed tocreate an awareness among the students towards what tobe accepted and what to be avoided during our choice of chemical processes and using chemicals. This course will also give insight to some advanced level of reagents that are being used in chemical transformations.

2A: Reagents in Organic synthesis 15M

One electron and two electron oxidants, Oxidations with Cr (VI): Jones oxidation, Collins oxidation PCC, PDC, PFC; DMSO based oxidations: Swern, Moffat, DMSO-SO_3 complex, DMSO-acetic anhydride, Hypervalent iodine oxidations: Dess-Martine periodinane, IBX, Iodobenzene diacetate; Oxidations with thalium nitrate, Ag_2O, RuO_4, OSO_4, $NaIO_4$.

Reduction with metal-hydrides of B, Al, Sn, Si. Dissolving metal-reduction, Synthetically useful hydrogenolysis reaction, Sm and In based reducing agents and enzymatic reductions.

2B: Green Chemistry 10M

Green chemistry-overview, twelve principles, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids, Microwave-induced organic reaction, Reactions by sonication, Solvent-free organic reactions.

Unit-3 30M

Course specific objective:

- To learn the fundamental principles and characteristics of LASER
- To learn the theoretical basis of spectroscopic selection rules in vibrational, rotational and Raman spectra

3A : Laser 15M

Principles of Laser and Maser action. Population inversion (two/three/four level systems). Basic elements in Laser, Characteristics of Laser Radiation, Single Mode and Tunable Laser, Harmonic generation, Applications.

3B : Theoretical Spectroscopy 15M

Transition probability and transition dipole integral. Selection rule. Einstein A, B coefficient, Selection rule for vibrational spectroscopy, anharmonic correction by perturbation, appearance

of overtones, selection rule for rotataional spectra, nuclear spin and rotational energy levels, Stark effect, Raman scattering, Selection rule for rotational, vibrational Raman effect

ELECTIVE/SPECIAL PAPER (Paper XII)

Inorganic Chemistry

Course Specific Objective : This course will be advanced level course comprising of some topics of modern inorganic chemistry. Application of group theory in inorganic complex chemistry will be discussed and students will get familiar with transition of different levels and MO representation followed by advanced level magnetic chemistry. This will be helpful to the student to predict about the magnetic property of an unknown compound and the different transitions involved leading to a particular colour of the compound. An advanced level chemistry dealing with metalloenzymes chemistry and DNA interaction with an incoming ligand will help the students to predict the way of interaction of an unknown compound. Students will also get an idea to establish the probable structure of a metal complex by analyzing different spectroscopic data like IR, Uv-vis, Mossbauer, NMR, ESR etc.

Unit 1: Group Theory **20M**

Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, correlation diagram, Tanabe-Sugano diagram. Effect of lowering of symmetry on the orbitals and energy levels, correlation table. Justification of Laporte selection rule, vibronic coupling and vibronic polarization, polarization of electronically allowed transitions. Symmetry adapted linear combinations (SALCs) and the M. O. description of organic, inorganic and organometallic molecules.

Unit 2: Magneto chemistry **20 M**

Magnetic properties of transition metal compounds: Types of magnetic materials. Magnetic susceptibility and its determination: Gouy, Faraday methods , vibrating sample magnetometer, SQUID and NMR methods. Magnetic anisotropy, diamagnetism in atoms and polyatomic systems, Pascal's constants. Spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, temperature dependence of magnetic moment, spin cross over, Lande interval rule, energies of J states. Curie equation, Curie law and Curie-Weiss law.
First order and second order Zeeman effects, temperature independent magnetism, simplication and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes in cubic and axially symmetric crystal fields, low spin-high spin crossover.

Unit 3:Advanced Bioinorganic Chemistry 3 **20 M**

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer. Different possible ways of DNA interaction.

Metalloproteins catalyzing oxygen atom transfer reactions: Iron systems such as cytochrome P-450, methane monooxygenase, catechol and other dioxygenases, etc.
Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase; molybdo enzymes: xanthene oxidase, nitrate reductase, sulfite oxidase including some model study.
Other selected metalloproteins of various metal ions. Biological function of nonmetallic elements (other than C, H, O, N, S, P). Interaction of metal ions with bioligands.
Structural/functional models of some of the above mentioned systems.
Vitamins and coenzymes: Vitamin B_6 and vitamin B_{12} coenzymes, model systems

Unit 4: Spectroscospic Analysis of Inorganic Compounds 20M

Application of IR, UV, NMR, ESR, Mossbauer spectroscopy in inorganic chemistry (examples with simple and complex inorganic compounds including organometallic and cluster compounds and bio inorganic system).
Solid state reactions: Kinetics of solid state reactions by TGA, DTA and DSC methods (typical examples)

Organic Chemistry

Course Specific Objective :

This course will help the PG-students towards the understanding of advanced level of learning of stereo chemical aspects of organic molecules, their studies and their features that could be rationalised using pertinent measurement techniques. This portion is to enable to understand the ideas behind action of drugs in our body, SAR studies. The advanced level insight related to important heterocyclic motifs and NMR studies and application towards drug screening, MRI will also be introduced to the students.

Unit 1 : 20M

Stereochemistry: 10M

Advanced course involving conformation and reactivity, cyclic system, monocyclic systems- 3 to 10 member rings,6-6,6-5, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-6, 5-5-5 tricyclic systems. Chiroptical properties of organic molecules: origin, theory of CD, ORD principles and applications, Haloketone rule, Sector rule, Helicity rule, Exceptions and excitation chirality, Atomic and conformational asymmetry, Chiral analysis by polarimeter, NMR,GC, HPLC and capillary eletrophorasis methods, Baldwin rules-applications.

Advanced Pericyclic Chemistry: 10M

General perturbation molecular orbital theory in cycloaddition reaction: Reactivity, Regioselectivity and Periselectivity, Cheletropic reactions, 1,3-dipolar cycloaddition, Cycloadditions involving more than six electrons, Three and four component cycloaddotion, Ene reactions, Group transfer reactions and eliminations, Electrocyclic reactions of charged systems, Sigamatropic rearrangement: [1,5] and [1,7] shifts in neutral systems and [1,4] shift in charged

species, [3,3] shifts, Cope rearrangements, Claisen rearrangement, [5,5] shifts, [2,3] shifts in ylides.

Unit-2: **20M**

Medicinal Chemistry:

Pharmacodynamics: Different types of drugs and drug targets, Drug binding forces, Role of enzymes, Drug receptor interactions, Mechanism of drug action, Agonists, Antagonists, Affinity, Efficacy and potency of drug, Dose response curves.

Pharmacokinetics: Drug absorption, Distribution, Metabolism (Phase-I and Phase-II transformations), Excretion, Drug formulation and others.

Drug design and synthesis, Molecular and Quantum mechanics, Drawing chemical structures, equation and diagrams, 3D structures, Molecular modeling and energy minimisation, Molecular properties, Conformational analysis, docking procedures, *De Novo* design, Molecular recognition, Receptor based molecular modeling, QSAR studies, Antineoplastic agent, Cardiovascular drugs, Local anti-infectaive drugs, Antimalarial, antibiotics, anticolenergic and CNS active drugs.

Unit-3: **20M**

Heterocycles:

Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles; Heterocycles inorganic synthesis-Masked functionalities, Umpolung, Stork amination reation, Rearrangement and ring transformation involving 5-, 6- membered heterocycles with one hetero atom General approach to heterocycle synthesis, cyclisation, cycloaddition route.
Synthesis and reactions of aziridines, azitidines, oxazoles, thiazoles, imidazoles, isoxazoles, isothiazoles, pyrazoles and higher azoles and corresponding few systems, pyrimidines, pyridazines, pyrazines, purines, pteridines, Role of heterocyclic compounds in biological systems, Nomenclature of bicyclic and tricyclic fused systems, Introduction to the chemistry of azipines, oxepins, thiepins and their aza-analouges, Phosphorus and selenium containing heterocycles, Cyclazines.

Unit-4: **20M**

NMR Spectroscopy:

Introduction to Vector model (Bloch vector model) of NMR: Pulse technique (90^0 x pulse), FID, Multiple Pulses. Relaxation Process: Longituidinal relaxation, Transverse relaxation, Field Inhomogenity (T_1, T_2, T_2^*), 2D NMR, Corelation spectroscopy, Application of DEPT, ^1H-^1H COSY, HMBC, HMQC, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, reaction monitoring etc., Solid state NMR (CP-MAS).

Physical Chemistry

Course Specific Objective :

- To learn perturbation theories for application in simple systems, Stark effect on rotational spectra
- To learn advanced theories of statistical mechanics for application to rate processes and transport problems.
- To learn non-equilibrium treatment of thermodynamics
- To learn various aspects of photophysics and fluorescence spectroscopy of organic dyes
- To learn about polymers and nanomaterials

Unit 1 : Advanced Quantum Mechanics 16M

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications, Brillouin-Wigner theory, WKB method, Degenerate perturbation theory, Stark effect, First and second order lifting of degeneracy, Time-dependent perturbation theory, Derivation of Fermi's golden rule, Hellman-Feynman Theorem.

Unit 2 : Statistical Mechanics 3 16M

Einstein's theory of Brownian motion, Langevin equation, Fokker-Planck equation, Fluctuation-dissipation relation, effect of friction. Applications to rate processes and transport problems. Master equation and its applications.

Unit 3 : Non-equilibrium thermodynamics 16M

Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, balance equations for irreversible processes, Phenomenological equations, microscopic reversibility and Onsager reciprocity relations, examples and illustrations. , Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena, Some important applications.

Unit 4 : Advanced Photophysics 16M

Photophysics of unimolecular processes, Delayed fluorescence, Concentration dependence of quenching and excimer formation, Exciplex formation, Twisted intramolecular charge transfer processes, Excited state electron transfer processes, Marcus theory of electron transfer processes, Excited state intramolecular and intermolecular proton transfer reactions, Solvent relaxation dynamics, Forster resonance energy transfer (FRET) and its applications, Laser spectroscopic techniques of studying ultrafast reactions

Unit 5 : Modern Material Chemistry 16M

Electrically conducting polymers: Discovery of electrically conducting polymers, Factors affecting the conductivity of conducting polymers. Electrochemical polymerization. Doping of conducting polymers. Important structural features. Nature of charge carriers in conducting polymers: solitons, polarons and bipolarons. Mechanism of conduction in polymers. Electronic structure of polymers: Band theory of polymers. Methods for determining band structure of

polymers: An introduction. Nanomaterials : Hybrid materials as a new tool in material synthesis – advantages and applications. Biomedical applications of nanomaterials – drug delivery.

Project Work:
(Inorganic/Organic/Physical Spl.) Full Marks = 80 **6 credits ??** **Duration : 8 week**

Course Specific Objectives :

- To apprise the students about pursuing research after completion of Masters in chemistry
- To train them about choosing a research problem and pursuing it successfully

Unit-1: 50M

Research problem has to be finalized in consultation with the project supervisor. The work has to be carried out under the supervision of the project supervisor and Research Report of approximately 25 pages has to be submitted.

Unit-2 : 10M

The supervisor would send to the Department his/her assessment of the performance of the student in a sealed envelope.

Unit-3 : 20M

Seminar Lecture has to be delivered on the total work carried out. It will involve a Power Point Presentation (Total number of slides = 10; total presentation time = 10 minutes (max.) followed by questionnaire from the board of examiners having one external expert from outside the University