West Bengal State University

Department of Chemistry

Syllabus for M.Sc. in Chemistry

Under Choice Based Credit System (CBCS)

(Semester Programme)

[w.e.f. 2019-20 session]

Programme Specific Outcome

The purpose of the postgraduate programme in chemistry at West Bengal State University is to provide a firm foundation and prepare students for careers as professionals in the field of chemistry and the chemical industry. Students graduating with M.Sc. in chemistry will have an understanding of the fundamentals of chemistry in areas of Inorganic & Analytical, Organic and Physical Chemistry. He should be able to extend his knowledge in application areas of current chemical and scientific theories and research. The course will equip the students 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 the higher education institutes.

The course has been so designed such that the students would be able to independently design and carry out scientific experiments as well as accurately record and analyze the results of such

experiments. They are trained to be reasonably skilled in problem solving, critical thinking and analytical reasoning as required for scientific problems.

The research component will allow the students to develop the ability to explore new areas of research in both chemistry and allied fields of chemistry. They should learn to function as a member of an interdisciplinary problem solving team involved in inter-disciplinary research.

COURSE STRUCTURE

Semester	I	II	III	IV	Total Marks
Credit	22	22	24	24	92
Marks	300	300	300	300	1200
Course Type	Theo Pract	Theo Pract	Theo Pract	Theo Lab	
Core	150 100	150 100	150 50	120 30@	850
DSE			50$	80# 70	200
AECC	50 (Mixed)				50
SEC		50 (Mixed)			50
GE (for other subject students)			50		50

$: Spectroscopy/Analytical

#: Physical/Inorganic/Organic + Literature Review

@ Laboratory Related Assignment

The experiments detailed in the syllabus are indicative in nature. The specific experiments can be changed subject to available infrastructural conditions. The department will endeavor to introduce new protocols with advancement of the discipline.

SEMESTER I

Marks 300

Total Credit Points (CP) : 22

Course Code	Course Type	Course Taught	Marks	Total
	CHEM		Theo Pract	
CEMPCOR01T	Theory (Inorganic)	• Chemistry of coordination compounds I • Solution equilibrium of complexes • Bioinorganic chemistry I • Symmetry and Bonding	50	50 (CP = 4)
CEMPCOR02T	Theory (Organic)	• Theory and Methods in Structure-activity Relationship • Mechanism and Reactive Intermediates in Organic Chemistry • Pericyclic Reactions	50	50 (CP = 4)
CEMPCOR03T	Theory (Physical)	• Quantum Mechanics- I • Symmetry & Group Theory • Chemical Kinetics-I • Spectroscopy	50	50 (CP = 4)
CEMPCOR04P	Practical	• Inorganic + Physical	50	50 (CP = 4)
CEMPCOR05P	Practical	• Organic	50	50 (CP = 4)
CEMPAEC01M	Mixed	• Computer Language	50	50 (CP = 2)

SEMESTER II

Marks 300

Total Credit Points (CP) : 22

Course Code	Course	Course Taught	Marks		Total Marks
	CHEM		Th	Pr	
CEMPCOR06T	Theory (Inorganic)	• Chemistry of coordination compounds II • Different methods applicable for Electrochemical analyses • Bioinorganic Chemistry II	50		50 (CP = 4)
CEMPCOR07T	Theory (Organic)	• Nuclear Magnetic Resonance Spectroscopy • Asymmetric Synthesis in Organic Chemistry • Synthetic Strategy • Some Aspects of	50		50 (CP = 4)
CEMPCOR08T	Theory (Physical)	• Mathematics for Chemistry and Quantum Mechanics II • Macromolecules • Statistical Thermodynamics I • Electrochemistry 1	50		50 (CP = 4)
CEMPCOR09P	Practical	• Inorganic		50	50 (CP = 4)
CEMPCOR10P	Practical	• Organic + Physical + GV (25 +15+10)		50	50 (CP = 4)
CEMPSEC01M	Mixed	• Chemical & Spectral Analysis	50		50 (CP = 2)

SEMESTER III

Marks 300

Total Credit Points (CP) : 24

Course Code	Course Type	Course Taught	Marks		Total
	CHEM		Th	Pr	
CEMPCOR11T	Theory (Inorganic)	• *f*– Block Elements: Lanthanide and Actinide Elements • Crystallography • Nuclear Chemistry & Radiochemical Analysis • Chemistry of d-	50		50 (CP = 4)
CEMPCOR12T	Theory (Organic)	• Organometallic Chemistry • Synthetic Methodology • Photochemistry • Natural Products	50		50 (CP = 4)
CEMPCOR13T	Theory (Physical)	• Quantum Mechanics III • Nanomaterials • Statistical Mechanics II • Electrochemistry II	50		50 (CP = 4)
CEMPCOR14P	Practical	• Physical		50	50 (CP = 4)
CEMPDSE 01T	Theory [Spectroscopy or Analytical Chemistry]	**Spectroscopy** • Mass & IR spectroscopy • Emission spectroscopy • Mossbauer spectroscopy & Photoelectron spectroscopy • Electron spin resonance spectroscopy **Analytical Chemistry** • Fundamentals of Chemical Analysis • Solvent Extraction and Concept of Chromatography	50		50 (CP = 4)
CEMPGEC01T	Theory (for other departments)	• Spectroscopy Fundamentals • Thermodynamics • Crystal Field Theory • Reaction Mechanisms	50		50 (CP = 4)

SEMESTER IV

Marks 300

Total Credit Points (CP) : 24

Course Code	Course Type	Course Taught	Marks Th	Marks Pr	Total Marks
CEMPCOR15T	(Inorganic + Lab Quiz)	• Inorganic Rings, Cages and Clusters • Inorganic Reaction Mechanism	40	10	50 (CP = 4)
CEMPCOR16T	(Organic + Lab Quiz)	• Reagents in Organic synthesis • Heterocycles • Medicinal Chemistry •	40	10	50 (CP = 4)
CEMPCOR17T	(Physical + Computer Lab)	• Quantum Mechanics and Spectroscopy • Laser • Non-equilibrium thermodynamics • Bio-physical	40	10	50 (CP = 4)
CEMPDSE02T	Theory [Inorganic or Organic or Physical]	Inorganic • Magneto chemistry • Advanced Bioinorganic Chemistry 3 • Spectroscopic Analysis of Inorganic Compounds • Chemical application of group theory Organic • Advanced	50		

		Chemistry • Stereochemistry II • Advanced NMR Spectroscopy • Carbohydrates Physical • Advanced Quantum Mechanics • Statistical Mechanics III • Material Chemistry • Advanced		
CEMPCOR18M		• Research Project	30@ 70$	100 (CP=8

@Literature Review (in any area of choice) $ Project Work + Grand Viva

Semester I

CEMPCOR01T
Inorganic Chemistry- 1

Course Specific Outcome:

This course is designed to introduce the students to the basic inorganic chemistry of PG level. Some 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 processes and role of metalloenzymes in vivo. The concepts that were dealt with qualitative approach like VB theory and MO theory will be established by theoretical calculations.

Unit 1 : Chemistry of coordination compounds I **13M**

Crystal field 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 2 : Solution equilibrium of complexes 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 3 : Bioinorganic chemistry I **13M**

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-4 : 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, Bonding in homo-nuclear and heteronuclear diatomic molecules of 2nd period. Bonding in triatomic (H_3^+ , BeH_2, H_2O), tetraatomic (BH_3, NH_3), CO, NO and CH_4. MO diagrams. Huckel – pi – electron theory and its applications to ethylene, allyl, butadiene and benzene, idea of self consistent field. Concept of resonance.

CEMPCOR02T
Organic Chemistry-1

Course Specific Outcome :

The students will be introduced to the basic theoretical methods and calculations that are involved in assuming and proving various organic molecular properties *viz.* aromaticity, acidity-basicity, reactivity, rate of reactions *etc*. This will impart a thorough knowledge about the mechanisms of reactions which will help them to detail understanding of a course of a reaction. The students would also be introduced to higher level of learning of stereochemical phenomena, their application towards the understanding to pericyclic and other reactions of organic molecules. The knowledge of new class of pericyclic reaction is another thrust area. This will impart basic idea of interaction between MO(s) and the concept of atom efficiency will be introduced too.

Unit 1 : Theory and Methods in Structure-activity Relationship **13M**

The Huckel MO: Theory, Method and Application to acyclic and cyclic conjugated systems - ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene. Huckel's rule and concept of aromaticity, alternant and non-alternant hydrocarbons, anti aromaticity, pseudoaromaticity, homo-aromaticity. Criteria of aromaticity of annulenes, heteroannulenes, fullerenes (C_{60}) *etc.*
Frost diagram: Concept, formation and application related to aromatic property.
Linear Free Energy Relationship for substituent effect: Hammett equation and its modifications.

Unit 2 : Mechanism and Reactive Intermediates in Organic Chemistry **12M**

Determination of organic reaction mechanism, Isolation and Identification of intermediates, Trapping of Intermediates, Isotopic labeling, Stereochemical evidence, Kinetic evidence, Hard and soft acids and bases.

Reactive intermediates – Formation and stability of classical and non classical carbonium ions, Carbanions, Carbenes, Arynes, Nitrenes. Radical: Production, Characteristics, Substitution, Addition and Elimination reactions.

Unit 3 : Pericyclic Reactions **13M**

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, Cope and Claisen rearrangements. Ene reaction.

Unit 4 : Stereochemistry-I **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

CEMPCOR03T

Physical Chemistry-1

Course Specific Outcome :

The students will primarily sharpen the concepts that they have learnt in the undergraduate classes with new extension and applications. Major focus in this semester will be on the four fundamental areas of quantum mechanics, group theory, kinetics and spectroscopy. Major thrust will be on the basic concepts and theories that have lead to the development of the four different areas as mentioned above.

Unit 1 : Quantum Mechanics-I **13M**

Postulates of quantum mechanics and their analysis; Properties of operators and commutators; Time-independent Schrodinger equation; Concept of stationary states, Free particle, Particle in a one dimensional box, Barrier problems and tunneling phenomenon ; Equation of motion; Ehrenfest's theorems, Angular momentum operators, Eigenvalues and eigenfunctions, Hydrogen atom Problem: Cartesian and Polar coordinates. Centre of Mass and relative coordinate, Spherical harmonics. Real and complex orbital, Role of the constant of motion.

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 : Chemical Kinetics-I **13M**

Collision theory and activated complex theory. Reactions between ions: influence of solvent dielectric constant (double sphere model), single sphere activated complex model, influence of ionic strength. Unimolecular reactions. Chain reactions. Kinetics of fast reactions: flow method, relaxation method, flash photolysis. Oscillatory reactions: Observation and mechanism. Autocatalytic reaction.

Unit 4 : 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. Stark Effect and determination of Dipole moment. Non-rigid rotor, Breakdown of Born-Oppenheimer approximation, vibrational-rotational spectra

CEMPCOR04P

Practical - 1

Inorganic Chemistry practical: **25M**

Course Specific Outcome :

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 etc.

(B) Complexometric Estimation of Fe(III) and Al(III) mixture, Cu(II) and Zn(II) mixture or other mixtures.

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

Physical Chemistry Practical **25M**

: Course Specific Outcome :

The students will learn to independently handle the basic equipments like spectrophotometer, potentiometer, pH-meter, and conductivity meter and carry out experiments using these instruments. The experiments have been so designed that they can verify the different fundamental laws and equations that they have learnt at the undergraduate level.

1. pH-metric titration of a polybasic acid and determination of its basicity and dissociation constants
2. Determination of Isoelectric Point of Gelatine
3. Determination of Solubility Product of PbI_2
4. Conductometric Titration of a Mixture of Halides (KCl + HCl + NH_4Cl) by i) NaOH and ii) $AgNO_3$
5. Spectrophotometric determination of pK_{In} of Bromocresol Green and determination of Isosbestic point.
6. Potentiometric Titration of (KI+KCl) by $AgNO_3$ solution.
7. Determination of E_o of the Quinhydrone electrode by potentiometric method
8. Determination of Hydrolysis Constant of a Salt With the Help of a pH-meter

CEMPCOR05P

Practical - 2

Organic Chemistry Practical **50M**

Course Specific Outcome :

This part of the course is so designed to make the PG students able to analyse the organic compounds. They will learn to separate various mixtures of functionalised organic compounds on the basis of solubility and re- crystallize them accordingly. The students will study their physical and chemical properties and thus by identifying different organic molecules they will be able to get hand on experience related to their so far gathered theoretical knowledge. Also, by means of preparing relevant derivatives the students would be introduced to the understanding of nature of different chemicals and reaction conditions and thereby they will be able to develop their skills towards different organic transformations. Students will learn synthetic methodologies towards a few organic compounds along with their spectral characterization by

UV-Vis and IR. Green methodologies are introduced to the students to impart the knowledge of sustainable chemistry.

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(A) Identification of individual organic compounds from the mixture of two solid compounds:

- Separation on the basis of solubility
- Detection of functional group(s) present in each constituent organic compound (not more than one functional group in a component)
- Preparation of derivative
- Determination of melting points of the separated organic compounds.
- Determination of the melting point of the derivatives.
- Identification of two solid compounds individually by means of checking melting point of the compounds and their corresponding derivatives with the help of the melting points reported in literature.

(B) Some Single-step organic synthesis/transformation including few Green methods.

1. Bromination of acetanilide to p-bromoacetanilide,
2. Photoinduced transformation of benzophenone to benzopinacol,
3. Base promoted hydrolysis of methyl salicylate,
4. Rearrangement without using organic solvent: Benzil to benzillic acid (in Solid phase). *etc.*

CEMPAEC01M

Course Specific Outcome :

Theoretical components have become a major part in physical chemistry research as well as understanding the new softwares for the different applications which are needed for data analysis in current day research in chemistry. The objective of this course is to make the students capable to write such computer programs which will give them the required expertise in this field.

Computer Programming 50M

Semester II

CEMPCOR06T

Inorganic Chemistry – 2

Course Specific Outcome :

In this course the students will learn some advanced topics in crystal filed theory and bioinorganic chemistry as a continuation of the earlier semester. 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. Solid state chemistry course will give an idea about band theory and introduce them to the field of superconductor. Slightly advanced level bioinorganic chemistry will be introduced keeping in mind mainly the different metalloenzymes present in vivo.

Unit 1: Chemistry of coordination compounds II **13M**

Electronic spectra of transition metal complexes : Microstates, determination of ground and excited state terms of d^1 to d^9 ions in octahedral and tetrahedral fields; 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 etc.).

Unit 2 : Different methods applicable for Electrochemical analyses **12M**

Use of three electrode system, standard electrodes and applications. Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry, Dropping mercury electrode, stripping voltametry

Unit 3: Bioinorganic Chemistry II **13 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.

Unit 4: Chemistry of 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, chemical and quantum mechanical concept, 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.

CEMPCOR07T

Organic Chemistry – 2

Course Specific Outcome :

This course is to enable the students to get the knowledge of the probably most powerful spectroscopic technique, NMR and its application to interpret the structural features of molecules. The deliverable knowledge to the students based on how the spectroscopic technique could be used to judge the purity, architectural features, and properties of compounds is the key idea behind this course. The Post Graduate students will also learn some important manifestation of asymmetric organic chemistry and its application in various chiral compound syntheses including some bio-active molecules. The targeted organic molecules synthesis including bio-active compounds has been found to be the area of interest to the synthetic chemists. The knowledge of the different perspective of such targeted synthesis based on disconnection approach is also included here. Some aspects of biomimetic chemistry and related topics are included here to impart the key understanding to the students about the intimate relationship of the chemical world with the various phenomena taking place in the living world.

Unit-1 : Nuclear Magnetic Resonance Spectroscopy **13M**

Basic Principle, Nuclear spin, Nuclear resonance, Basic instrumentation, FT-NMR (qualitative idea) and its advantages, Saturation, Chemical shift and its measurements, Shielding-deshielding, Factors influencing chemical shift, Spin-Spin interactions, Factors influencing coupling constant `J`. Classification of molecules: ABX, AMX, ABC, A_2B_2, *etc.*, Spin decoupling, first order and non first order spectra. Basic principle of NOE and its application, Concept of difference spectra, preliminary concept of COSY. Introduction to CMR: Basic idea. Sensitivity, Proton decoupled and non-decoupled CMR, Off Resonance CMR. Applications of NMR in medical diagnosis: Brief idea related to MRI.

Unit-2: Asymmetric Synthesis in Organic Chemistry **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,Alkeneisomerisation, Hydrolysis and esterification

Unit-3: Synthetic Strategy **13M**

Retro-synthetic analysis; Disconnection approach; Typical examples to illustrate the disconnection approach; FGI; Umpolung (1,3-dithiane);One-group, Two-group disconnections; Retron; Protection and deprotection of common functional groups (Hydroxy, Carbonyl, Carboxylic and Amino groups), Disconnection of some interesting organic compounds(alkaloid, well known drugs)

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

Molecular models of biological receptors and principle of molecular recognition, Biomimetic chemistry, Design, Synthesis and binding studies of synthetic receptors, Enzyme models: enzyme kinetics, inhibition, immobilsation and application, Micelles, Cyclodextrin, Remote functionalisation reaction, Biopolymers: Proteins, Peptides.

CEMPCOR08T

Physical Chemistry-2

Course Specific Outcome :

The course has been designed in such a manner that here the students are introduced to the mathematical concepts with application to chemistry both from quantum mechanical as well as statistical mechanical angles. Electrochemistry a fundamental area of chemistry is introduced to the masters students in this semester so that the students find answers to the different chemical phenomenon they see around them. Polymers have become a part of our daily existence. In this semester the students are given a brief introduction to the topic with some advanced knowledge which will guide them if they want to study the subject in the future.

Unit-1: Mathematics for Chemistry and Quantum Mechanics II **13M**

Elements of calculus, Extremum principles, constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier series. Vectors and linear vector space: matrices. Applications. Particle on a ring, Rigid Rotor, 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 (anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

Unit-2: Macromolecules **12M**

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. Biomacromolecules (Proteins & DNA).

Unit-3: Statistical Thermodynamics I **13M**

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, Application to chemical/ionization equilibrium.

Unit 4 : Electrochemistry I **12M**

Ion solvent interactions, Electrode surfaces-potential and measurements, Thermodynamics of such systems, Lippman equation, Gouy Chapman & Stern models. Debye Huckel theory and its extension. Debye Huckel Onsager theory and its extension. Photoelectrochemistry at surface solution interface, Photoelectrochemical splitting of water and carbon dioxide, waste reduction

CEMPCOR09P

Practical -3

Inorganic Chemistry Practical **50M**

Course Specific Outcome :

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. Interpreting skill and logical method of analysis of students would be augmented by means these studies. Modern day spectroscopic analysis will also be introduced so that the students can apply their knowledge to analyze the probable structure of synthesized metal complexes. 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.

Inorganic Practical

Part (A) **25M**

(1) 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

(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) 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.

Part-(B) **25M**

(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 ($CaCO_3$, $MgCO_3$, 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).

(2) Analysis of Mixture:

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

(3)Spectroscopic Studies on Model Compounds

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

CEMPCOR10P

Practical-4

Organic Practical **25M**

Course Specific Outcome

The students will have hands on training to extract and purify natural product(s) and to explain the structural features of the same based on spectroscopic data. The students will handle the instruments like UV, FT-IR *etc.* on their own and thus skills to handle modern instruments will be developed. Students will learn few multistep organic syntheses and thereby the skill of purification of compounds using column chromatographic technique will also be introduced to them.

(A) Extraction, purification and spectroscopic study of Natural Product.

1. Extraction of Caffeine from tea leaves (commercially available tea-bags) by solvent extraction method.
2. Determination of melting point.
3. Spectroscopic study of the extracted compound:
    - IR
    - UV
    - NMR
4. Purification:
    - Method of sublimation
5. Preparation of caffeine salicylate and determination of its melting point.

(B) Multi-step organic synthesis, their purification by column chromatography and structural studies based on some spectral data (maximum two synthesis).

Physical Chemistry **15M**

Course Specific Outcome

The objective of the practical course is to experimentally verify the different concepts that the students have learnt from their theoretical classes. The experiments require more attention and precision and the data interpretation becomes slightly more complex. This will teach the students to think and analyze their results before coming to a conclusion.

1. Kinetic study of the autocatalytic reaction between potassium permanganate and oxalic acid.
2. Spectrophotometric Study of the Alkaline Hydrolysis of Crystal Violet. (Determination of rate constant "k" and order "n" with respect to alkali)
3. Determination of equilibrium constant of acid hydrolysis of an ester.
4. Determination of Critical Micelle Concentration (CMC) of SDS by Conductometry
5. Potentiometric titration of acetic acid by sodium hydroxide using quinhydrone electrode.
6. Kinetic Study of the Iodination of Aniline by Colorimetric Method.
7. Verification of Onsager Equation and Determination of λ_0 and K_a of Acetic Acid

Grand Viva Examination **10M**

CEMPSEC01M

50M

Course Specific Outcome

Analysis of chemical sample forms a major component in chemistry. This course has been so designed that the students are given the knowledge to interpret the different data and identify and characterize the samples. This knowledge can be further used in terms of employment since all laboratories and research organizations need trained manpower for data interpretation and analysis. The department feels that this course will significantly add to the technical skill of the student.

(1) Elucidation of different methods of synthesis and characterization of inorganic and coordination compounds-some representative examples:

A. Polynuclear clusters reported in literature.

B. Mn12 Acetate.

C. Preparation of copper glycine complex-bis(glycinato)copper (II).

D. Preparation of N,N-bis(salicyldehyde)ethylenediamine, Co(salen)

E. Selected coordination compounds with some common inorganic and organic ligands and with bi-, tri- and polydentate N, O donor ligands, oximes etc; Complexation and purification of complexes; estimation of metal inos present in coordination complexes

(2) Parameters of water analysis

Procedure of analysis of BOD, COD, DO, TOC, TOD and similar parameters

(3) Spectroscopic analysis:

Basic idea of using UV, IR, NMR, MASS, ESR spectrometry and elemental analysis: Determination of empirical formula from elemental analysis, Determination of molecular formula using molecular mass of the compound, Systematic application of the spectral data to determine and confirm the structure of the molecule by interpreting the supplied and/or obtained spectral data, Application of the spectra to study and diagnose various molecular properties.

Semester III

CEMPCOR11T

Inorganic Chemistry – 3

Course Specific Outcome :

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. A detailed group chemistry is given here as well as a portion of lanthanides and actinides will be here so that students become familiar with elements having similar property.

Unit 1: *f*– Block Elements: Lanthanides and Actinides 13M

:

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.

Unit 2: Crystallography 12M

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 3: Nuclear Chemistry & Radiochemical Analysis 13 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 4: Chemistry of d-Block Elements **12M**

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.

CEMPCOR12T

Organic Chemistry – 3

Course Specific Outcome :

This portion is to develop the basic concepts of designing an organic molecule that is heavily dependent on the proper choice of various reagents. The knowledge of usage of specific organic reagents of some main group elements is introduced here. Accordingly, some advanced level of information of organo-main group reagents and reactions involving organometallic chemistry are incorporated here. This course is also to impart the knowledge of understanding to the students of a special type of method and mechanism of photochemical transformation. The students will be introduced to some naturally occurring macromolecules, their structural features and the challenges towards their synthesis.

Unit-1: Organometallic Chemistry **13M**

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: Synthetic Methodology **12M**

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

Organophosphorus: Chemistry of organophosphorus compounds; Phophorusylides; Wittig reaction and its modofications; Chiralphosphines; Phosphine-oxides and its applications.

Organosulphur: Chemistry of organophosulphur compounds, Sulphur stabilization of anions and cations, Sulphonium salts, Sulphonium and sulphoxoniumylides, Chiralsulphoxides

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

Unit-3: Photochemistry **13M**

Basic principles, Direct and sensitized reactions, Photochemistry of carbonyl compounds; Norish type-I and Norish type-II reaction; β-cleavage; Photo-oxidation and Photo-reduction; Photocycloaddition; Patterno-Buchi reaction; Photorearrangement(dienone); Photochemistry of olefinic compounds; Photoisomerisation(cis-trans isomerisation);Photocycloaddition; Di-pi methane rearrangement; Photochemistry of aromatic compounds.

Unit 4 : Natural Products **12M**

Terpenoids

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.

Alkaloids & Steroids

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

CEMPCOR13T

Physical Chemistry – 3

Course Specific Outcome :

The objective of the course is to introduce the students to slightly advanced quantum mechanical theories having relevance to chemical bonding, molecular properties and spectroscopy. The statistical mechanics course becomes more advanced and introduces the students to research in theoretical concepts of chemistry. The students will be introduced to nanomaterials, which give a new dimension to research in material science. In electrochemistry the students will learn the areas of electrode kinetics and corrosion.

Unit-1 : Quantum Mechanics III **13M**

Virial theorem and chemical bonding; Hellmann-Feynman theorem, Electrical responsive properties; Time-dependent perturbation theory, Derivation of Fermi's golden rule, Harmonic perturbation and transition probabilities.

Unit-2 : Nanomaterials **12M**

Nanomaterial- definition and properties, relevance to dependency on size and shape. Synthetic methodologies both physical and soft chemical methods { i) mechanical methods, ii) Evaporation methods, iii) CVD, iv)Sol-gel, v) Micromulsion (normal and reverse micelles formation), vi) Template based synthesis, vii) reduction methods }. Various kind of Nanostructures; Quantum dot (QDs), Carbon Nanotubes, (SWCNT, MWCNT), Fullerene, Graphene, etc. Application of nanomaterials.

Unit-3 : Statistical Mechanics II **13M**

Phase space, ergodic hypothesis, Liouville's theorem, Concepts of different ensembles with applications to selective systems. Fluctuations. Perfect gas and the Sackur-Tetrode equation, System of interacting molecules, treatment of imperfect gases, Black body radiation.

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

Electrode kinetics-Nernst, Butler-Volmer equation, Tafel equation. Overpotential, polarography, Amperometric and coulometry titrations. Linear sweep voltametry, Cyclic Voltametry. Fuel cells. Corrosion – local cell theory, Pourbaix diagram and corrosion of Fe. Corrosion current and potential-Evans diagram, Corrosion control - cathodic, anodic, mixed, H_2 embrittlement. Stress corrosion, cracking corrosion, Measurement - weight loss, electrochemical and Stern Geary method.

CEMPCOR14P

Practical -5

Physical Chemistry **50M**
Course Specific Outcome

The objective of this course is to enable the students to think on their own, design or modify certain reaction conditions and try to analyze the result. In addition the students will also carry out slightly critical experiments which will sharpen their data interpretation aptitude.

1. Kinetic Study of the Inversion of Sucrose

2. Determination of the Standard Redox Potential (E_o) of Ferrocyanide – Ferricyanide System
3. Kinetic Study of the Reaction between $K_2S_2O_8$ and KI and study on the effect of Added salt on the Rate constant.
4. Studies on Kinetics of Iodination of Acetone.
5. Determination of the standard redox potential (E_0) of ferrocyanide-ferricyanide system.
6. 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.
7. Verification of the Onsager equation and Conductometric determination of Solubility Product of a sparingly soluble salt.
8. Determination of the Co-ordination number of copper in copper-ammonia complex.
9. Determination of the Standard Electrode Potential (E_o) of Ag/Ag^+ system and Activity Coefficient of Ag^+ ions in solution.
10. Determination of equilibrium constant for the formation of Iron (III) Thiocyanate complex.

CEMPDSE01T

ELECTIVE

Spectroscopy

Course Specific Outcome :

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: Mass & IR spectroscopy **13M**

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.

Unit-2 : Emission spectroscopy 12M

Franck-Condon principle, Mirror-image symmetry and its violation, Radiative and radiationless deactivation, Oscillator strength, Fluoroscence Quenchers and life-time variations, Photophysical processes of unimolecular processes, Delayed fluorescence, Kinetics of bimolecular processes: collision quenching, Stern-Volmer equation, Concentration dependence of quenching and excimer formation, Excited state electron transfer processes.

Unit-3: Mossbauer spectroscopy & Photoelectron spectroscopy 13M

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

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-4: Electron spin resonance spectroscopy 12M

Basic principles, Principle of EPR and spin Hamiltonian (comparison to NMR spectroscopy), external standard, line-width, nuclear hyperfine interactions, anisotropy in Lande g factor and hyperfine interaction, zero field splitting, and Kramer`s degeneracy, factors affecting the `g` value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities. Basic instrumentation, measurement techniques and simple applications regarding structural information of organic radical and inorganic molecules from EPR spectra..

Analytical Chemistry

Course Specific Outcome :

This course is designed to introduce the students to different methods of analytical chemistry. Different classical methods of analysis will be discussed along with basic aim of analytical chemistry. Solvent extraction and different chromatographic methods will give an idea of

modern day separation and purification techniques used in chemical industry. Moreover, kinetics of reactions will give students an opportunity to learn catalytic reactions.

Unit-1: Fundamentals of Chemical Analysis **13 M**

Aim of analytical chemistry. Standardization and calibration. Quality assurance and quality control. Process control and validation.

Classical methods of analysis: Gravimetry and titrimetry including neutralization, complexation and oxidation-reduction. Complex acid-base equilibrium. Separation of metal ions as their hydroxides, sulphides and chelates. Examples of gravimetric and complexometric analysis.

Unit-2: Solvent Extraction and Concept of Chromatography **12 M**

Liquid-Liquid extraction – Cross and counter current process, multiple batch extraction, solvent extraction of metal ion, solid-phase extraction. Classification of chromatographic separation. Aqueous biphasic and supercritical fluid extraction. Band broadening and column efficiency, Theoretical plate model and the Rate theory of Chromatography.

Unit-3: Liquid Chromatography and Other Types of Chromatography: **13 M**

Reverse and normal phase chromatography, gradient elution, solvent selection and classes, ion exchange and ion chromatography.

HPLC: Basic equipment, pumping and injection system, column stationary phase and structural types of column packing, Detector systems (UV, IR, Conductometric, Fluorescence), Sample preparation and applications.

Gas chromatography: gas-liquid and gas-solid chromatography, types of column and selection. Basic equipment, Injection systems, Detectors (FID, TCD, ECD, NPD) for GC, sample separation and applications. Characteristics and applications of Size exclusion Chromatography, Affinity chromatography, Supercritical Fluid Chromatography, Capillary Electrophoresis.

Unit- 4: Kinetics in Analytical Chemistry **12 M**

Significance of reaction kinetics in analytical chemistry. Determination of rate of fast reactions. Analytical application of catalytic and non-catalytic reactions in single species and pseudo single species systems. Differential reaction rate methods of analysis and its limitations, determination of inorganic and organic mixtures.

CEMPGEC01T
(for other disciplines)

Chemistry Fundamentals

Course Specific Outcome :

This course is designed for students undergoing postgraduate studies in WBSU other than those in the Chemistry department. This is an interdepartmental course which is open to students from all other disciplines. The idea of the course is to familiarize the students with the fundamental concepts of chemistry. Since research in science has become interdisciplinary in nature this course has been so designed that a student is introduced to the principles in the fields of spectroscopy, crystal filed theory, organic reaction mechanisms and thermodynamics. This knowledge should help students who want to pursue higher studies in allied disciplines.

Unit – I : Spectroscopy **13M**

UV Spectroscopy:

Introduction;types of electronic transitions, chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper/Hypochromic effects); application of Woodward's Rules for calculation of λ_{max}.

IR spectroscopy:

Basic principle, Characteristic vibrational frequencies of 'C=O' (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides and conjugated carbonyl compounds), 'O-H' and 'N-H', Effects of solvent, hydrogen bonding on vibrational frequencies, overtones.

Nuclear Magnetic Resonance Spectroscopy:

Basic Principle, Nuclear spin, Chemical shift and its measurements, Shielding-deshielding, Factors influencing chemical shift, Spin-Spin interactions, Factors influencing coupling constant `J`. Spin decoupling, first order and non first order spectra, Relaxation, Basic principle of NOE and its application, Concept of difference spectra, Introduction to CMR,Applications of NMR in medical diagnosis: Brief idea related to MRI.

Unit – II : Basic idea of crystal field theory **12M**

Valence Band theory, Basic idea of crystal filed theory, Splitting of d-orbitals octahedral and tetrahedral, square planar, fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environment, Octahedral site preference energy, spienel amd inverse spienel, hole formalism, inversion and equivalence reactions, splitting of d_n terms in octahedral and tetrahedral fields, Tetrahedral distortion and Jahn Teller effect. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy.

Unit – III : Classification of organic reactions and study of their mechanism 13M

1. Substitution Reactions
2.Addition Reactions
3.Elimination Reactions
4.Rearrangement Reactions
5.Oxidation Reactions
6.Reduction Reactions
7.Oxidative Coupling
8.Reductive Coupling

Unit – IV : Thermodynamics 12M

Introduction to thermodynamics- 1st and 2nd law of thermodynamics, Thermochemistry and its applications, Physical concept of Entropy and auxiliary state functions (G and A), criteria for spontaneity and equilibrium, application to biological systems.

Semester IV

CEMPCOR15T

Inorganic Chemistry – 4

Course Specific Outcome :

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. The course of organometalic chemistry will be introduced here. This portion will enable them to understand different kinds of bonding including η bonding.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.

Unit-1 : Inorganic Rings, Cages and Clusters **10M**

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.

Unit – 2 : Inorganic Reaction Mechanism **10M**

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 3: Organometallics **20M**

1 A

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

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).

1-B

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.

CEMPCOR16T

Organic Chemistry - 4

Course Specific Outcome :

This course will give insight to some advanced level of reagents that are being used in chemical transformations. The students will be introduced to the advance level of knowledge regarding the important heterocyclic organic compounds including some bio-active molecules. Chemicals and Chemistry are basically intimate part of our day to day life and lifestyle whether we name them as food or drug. Naturally, this portion of course is designed to impart some elementary ideas about what happens to a particular species as well as to our body when we take them and thereby to create awareness among the students towards what to be accepted and what to be avoided during our choice of foods and drugs. The Post Graduate students will also learn the host-guest chemistry which remains one of the interesting areas to be studied and explored by the organic synthetic chemists as well as by the biochemists.

Unit-1 Reagents in Organic synthesis 10M

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, Iodobenzenediacetate; 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.

Unit-2: Heterocycles 10M

Heterocycles in organic synthesis-Masked functionalities, Umpolung,6- membered heterocycles with two hetero atom General approach to heterocycle synthesis, cyclisation, cycloaddition route. Synthesis and reactions of pyrimidines, pyridazines, pyrazines, purines, pteridines.

Unit-3: Medicinal Chemistry **10M**

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, *De Novo* design, Molecular recognition, Receptor based molecular modeling, QSAR studies, Antineoplastic agent, Cardiovascular drugs, Local anti-infective drugs, Antimalarial, Antibiotics, Anticolenergic and CNS active drugs.

Unit-4: Supramolecular Chemistry **10M**

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

CEMPCOR17T

Physical Chemistry - 4

Course Specific Outcome :

This course has been designed so that the students learn the theoretical basis of spectroscopic selection rules based on time-dependent perturbation theory, principle of LASER and its function. Also the concept of non equilibrium thermodynamics and certain concepts of bio physical chemistry have been included in the syllabus. The objective of the course if to give the students an advanced understanding of the above concepts in physical chemistry

Unit-1: Quantum Mechanics and Spectroscopy **10M**

Theoretical basis of interaction of radiation with matter: Harmonic perturbation and transition probabilities, Selection rule for vibrational spectra, anharrmonic correction by perturbation - appearance of overtones, selection rule for rotational spectra, Raman scattering, Application of group theory to molecular vibrations, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule

Unit-2: Laser **10M**

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

Unit 3 : Non-equilibrium thermodynamics **10M**

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 : Bio-physical Chemistry **10M**

Configuration and conformation of biological macromolecules. Membrane structure. Spectroscopic methods : UV-Vis and CD. Separation techniques : Gel Electrophoresis. Macromolecule-ligand binding and cooperativity, Drug-DNA interaction.

CEMPDSE02T

ELECTIVE

Inorganic Chemistry

Course Specific Outcome :

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, CV, TGA, DTA and DSC, etc.

Unit 1: Magneto chemistry **13 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 2:Advanced Bioinorganic Chemistry III **12 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 3: Spectroscospic Analysis of Inorganic Compounds **13M**

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)

Unit 4: Chemical application of group theory **12M**

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.

Organic Chemistry

Course Specific Outcome :

This course will help the PG-students towards the understanding of advanced level of learning of stereo chemical aspects of organic molecules and their studies and their features hereby could be rationalised using pertinent measurement techniques. The advanced level insight related to pericyclic reaction and important carbohydrate motifs are introduced here. Advance level NMR studies including correlation spectroscopy and their application towards molecular structure determination, drug screening, MRI will also be introduced to the students.

Unit-1 :Advanced Pericyclic Chemistry 13M

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

Unit 2 : Stereochemistry-II 12M

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.

Unit-3: Advanced NMR Spectroscopy 13M

Introduction to Vector model (Bloch vector model) of NMR: Pulse technique (90^0 x pulse *etc.*), FID, Multiple Pulses. Relaxation Process: Longituidinal relaxation, Transverse relaxation, Field Inhomogeneity (T_1, T_2, T_{2^*}), 2D NMR, Correlation spectroscopy, Application of DEPT,^{1}H-^{1}H COSY, HMBC, HMQC, TOCSY, NOESY in structure elucidation of organic compounds, Reaction monitoring and Drug screening, Basic Idea of Solid State NMR (CP-MAS).

Unit-4: Carbohydrates 12M

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.

Physical Chemistry

Course Specific Outcome :

This course is for the students who want to study physical chemistry in future. Hence, the nature of the course is slightly advanced in nature. The topics covered under advanced quantum mechanics include non-degenerate and degenerate perturbation theory to simple systems and Hartree-Fock theory. In statistical mechanics application to some selected problems will be discussed. Recent research directions in material chemistry alongwith advanced photophysics form the rest of the course content. The objective of the course shall be fulfilled if the students undergo future research and studies in physical chemistry.

Unit 1 : Advanced Quantum Mechanics 13M

Section A : Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications, Degenerate perturbation theory, Stark effect, First and second order lifting of degeneracy

Section B : Antisymmetric principle and antisymmetrizer operator. Independent particle model (IPM). Hartee and Hartee-Fock (HF) Theories. HF method for closed shells:

Unit 2 : Statistical Mechanics III 12M

Formulation of Quantum statistical mechanics: pure and mixed states, density matrix, quantum Liouville theorem and its consequences, Quantum statistics and ensembles. The specific heat of electron gas, Debye theory, Bose-Einstein condensation.

Unit 3 : Material Chemistry 13M

Conducting Polymers - Introduction, Structure and Characteristics, Types of conducting polymer, Conduction Process in conducting Polymers and concept of Doping, Role of Polarons, Biplorons and solitons in conduction mechanism. Chemical and electrochemical methods of synthesis of conducting polymers – Applications of conducting polymer.

Hybrid materials : Chemical synthesis of dimensionally modulated nanocomposites, core shell nanostructured materials and structures resulting from self assembly of nanomaterials. Applications and advantages of such materials.

Nanotechnology in Drug Delivery: Introduction to Nano mediated Drug Discovery and Development, Drug delivery system, Nanoparticles in Drug delivery, Applications of Nanoparticle in Drug Delivery Targeting and Cancer Treatment, Application of Lipids, CNTs,

proteins, peptides, dendrimer, cyclodextrin, based organic nanoparticles in nanomedicine and drug delivery

Unit 4 : Advanced Photophysics **12M**

Excited state inter and intra molecular proton transfer reactions, Excimer and Exciplex formation Excited state electron transfer processes, Marcus theory of electron transfer processes. Forster resonance energy transfer (FRET) and its applications

CEMPCOR18M

Research Project

Course Specific Outcome :

Students will obtain first hand experience of pursuing research during the postgraduate course and will be able to choose independently a research problem and try to solve 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 a report of the work done and the data collected during the course of his study of approximately 25 pages has to be submitted. Evaluation will be carried out on the work done, methodology of analysis of problem, supervisors assessment and defense in a seminar presentation by a panel of experts.
Time allotted : 8 weeks

Unit-2 : **30M**

The candidate is required to do a theoretical review of any topic of his choice in chemistry, prepare a report of the same of approximately 10 pages and present his observation in the form of a Seminar Lecture where his assessment of the review topic will be carried out by a panel of experts.

Unit 3 : Grand Viva Examination **20M**