COOCH BEHAR PANCHANAN BARMA UNIVERSITY

Syllabus for Post Graduate Course in Chemistry

(W.E.F. 2015)

SYLLABUS for M.Sc in CHEMISTRY

(Course Duration : Four Semester – Two Year)

Total Credit : 80 Credit per Semester : 20

Total Marks = 1600 Theory = 900 Practical = 300 Cont. Evaluation = 320 Attendance = 80

First Semester :

Course No.	Name of Course	Marks				Credit
		SE	CE	A	Total	
101	Organic Chemistry-I	75	20 (Class Test)	5	100	5
102	Inorganic Chemistry-I	75	20 (Class Test)	5	100	5
103	Physical Chemistry-I	75	20 (Class Test)	5	100	5
104	Practical –I (ORG+ING+PHY)	75 (25+25+25)	20 (CV)	5	100	5

Second Semester:

Course No.	Name of Course	Marks				Credit
		SE	CE	A	Total	
201	Organic Chemistry-II	75	20 (Class Test)	5	100	5
202	Inorganic Chemistry-II	75	20 (Class Test)	5	100	5
203	Physical Chemistry-II	75	20 (Class Test)	5	100	5
204	Practical –II (ORG+ING+PHY)	75 (25+25+25)	20 (CV)	5	100	5

Third Semester :

Course No.	Name of Course	Marks				Credit
		SE	CE	A	Total	
301 – 304 (A or B or C)	Special Papers (Any one from A, B and C)					
301-A	Organic Chemistry-III	75	20 (Class Test/CV)	5	100	5
302-A	Organic Chemistry-IV	75	20 (Class Test/CV)	5	100	5
303-A	Organic Chemistry-V	75	20 (Class Test/CV)	5	100	5
304-A	Practical : Organic-III	75	20 (Project/Seminar)	5	100	5
301-B	Inorganic Chemistry-III	-	-	-	-	-
302-B	Inorganic Chemistry-IV	-	-	-	-	-
303-B	Inorganic Chemistry-V	-	-	-	-	-
304-B	Practical : Inorganic-III	-	-	-	-	-
301-C	Physical Chemistry-III	-	-	-	-	-
302-C	Physical Chemistry-IV	-	-	-	-	-
303-C	Physical Chemistry-V	-	-	-	-	-
304-C	Practical : Physical-III	-	-	-	-	-

Fourth Semester :

Course No.	Name of Course	Marks				Credit
		SE	CE	A	Total	
401 – 404 (A or B or C)	Special Papers (A or B or C, as in 3rd Semester)					
401-A	Organic Chemistry-VI	75	20 (Class Test/CV)	5	100	5
402-A	Organic Chemistry-VII	75	20 (Class Test/CV)	5	100	5
403-A	Organic Chemistry-VIII	75	20 (Class Test/CV)	5	100	5
404-A	Practical : Organic-IV	75	20 (Project/Seminar)	5	100	5
401-B	Inorganic Chemistry-VI	-	-	-	-	-
402-B	Inorganic Chemistry-VII	-	-	-	-	-
403-B	Inorganic Chemistry-VIII	-	-	-	-	-
404-B	Practical : Inorganic-IV	-	-	-	-	-
401-C	Physical Chemistry-VI	-	-	-	-	-
402-C	Physical Chemistry-VII	-	-	-	-	-
403-C	Physical Chemistry-VIII	-	-	-	-	-
404-C	Practical : Physical-IV	-	-	-	-	-

SE: Semester Examination; CE: Continuing Evaluation; CV: Comprehensive Viva Voce; A: Attendance.

Course Content

Organic Chemistry

Semester – I

Course No. 101

A: Structure Activity Relationship

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

B: Stereochemistry – I

Acyclic systems up to 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 cyclohexene, decalins and their derivatives; Effects of conformation on reactivity in acyclic compounds and cyclohexanes. Elements of Symmetry and Chirality, Optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

C: Substitution (aliphatic electrophilic & nucleophilic) & Elimination reactions

Phase transfer catalysis; ultrasound, ambient nucelophile, regioselectivity.

D: Pericyclic Reaction

Classification and stereochemical modes. Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheleotropic reactions. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Hückel systems, Sommelet-Hauser, Cope, aza Cope and Claisen rearrangements , Ene Reaction, Wittig rearrangement, suitable examples of [(2Π +2 Π), (4Π +2 Π), (4Π + 4Π), (2Π +2 Π +2Π)] and metal catalysed cycloaddition reactions.

E: Spectroscopy – I

Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin decoupling, spin tickling, classification of ABX, AMX, ABC, A_2B_2 in proton NMR. Elementary principles of ESR, EPR and mass spectral techniques.

F: Natural Products – I

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

Course No. 104(Organic)

Practical : Identification of single organic liquid with one or more functional groups : purification of organic sample by distillation / vacuum distillation / fractional vacuum distillation, determination of boiling point, solubility analysis and classification, functional group analysis, derivatization and complete identification, use of spectroscopic techniques (IR, UV, NMR).

Semester – II

Course No. 201

A: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomerisation, stereomutation Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection (ESR) of radicals, radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, autooxidation.

B: Synthetic Strategy

Retrosynthetic analysis, disconnection approach, Typical examples to illustrate the disconnection approach, Functional group interconversion, Umpolung (1,3-dithiane), Convergent synthesis.

C: Synthetic Methodology

Organoboron – Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates.

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig, Stobbe reaction, hydrolysis of esters and amides, ammonolysis of esters, addition to C - C & C - N multiple bonds.

D: Spectroscopy - II

Introduction to ^{13}C NMR spectroscopy; theoretical treatment of rotational, vibrational and electronic spectroscopy, principles of photoelectron spectroscopy. Application of electronic, vibrational, NMR, ESR, EPR and mass spectral techniques to simple structure and mechanistic problems.

E: Stereochemistry – II

Correlation of axial dissymmetry and centrodissymetry, nomenclature of compounds involving axial and planar chirality, dynamic stereochemistry.

F: Reaction Kinetics & Mechanism

(a) Labelling and Kinetic isotope effects, Hammett, Hanch and Taft equations, sigma-rho relationship ,

Non classical carbonium ions.

(b) Thermodynamic & kinetic requirement, kinetic & thermodynamic control.

G: Natural Products – II

Familiarity with methods of structure elucidation (chemical & spectroscopic method), biosynthesis, synthesis and biological activity of the alkaloids - nicotine, atropine, coniine and papaverine.

Course No. 204 (Organic)

Practical :

Organic preparation involving aldol condensation, aromatic substitution reaction, Sandmeyer reaction, Friedel-Crafts reaction.

Quantitative analysis - Estimation of Phenol, Glucose & Sucrose. Determination of pk_a of benzoic acid.

Semester - III

Course No. 301-A

A: NMR Spectroscopy

Introduction to the techniques and Application of NMR: ^{1}H and ^{13}C NMR - principles, instrumentation; principles of decoupling, gated and inverse gated decoupling, NOE, relaxation process, selective polarization transfer, INEPT, basic two-dimensional sequence, homonuclear and heteronuclear shift correlation.

B: Heterocyclic Chemistry – I

Synthesis and reactions of aziridines, azetidines, oxazoles, thiazoles, imidazoles, isoxazoles, isothiazoles, pyrazoles and higher azoles and corresponding fused systems ; Nomenclature of bicyclic and tricyclic fused systems ; Introduction to the chemistry of azepins, oxepines, thiopins and their aza analogues; Phosphorus and selenium containing heterocycles, Cyclazines.

C: Medicinal Chemistry

Vitamins – General study, structure and synthesis of Vitamin A, Vitamin B complex, Vitamin C, Vitamin K, Vitamin D, Vitamin B, Biotin.

Course No. 302-A

A: Oxidative processes and Reductive processes

Introduction to different oxidative processes: Hydrocarbons -alkenes, aromatic rings, saturated C-H groups (activated and unactivated), Alcohols, diols, aldehydes ketones, ketals and carboxyalic acids, Amines, hydrazines, and sulphides

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

Introduction to different reductive processes: Hydrocarbons – alkanes , alkenes, alkynes and aromatic rings.

Carbonyl compounds: aldehydes, ketones, acids and their derivatives, Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis.

B: Rearrangement / Selective Organic reactions

Shapiro, Sharpless asymmetric epoxidation, Ene reaction, Barton reaction, Hofmann - Loffler – Freytag reaction.

C: Stereochemistry – II

Chiroptical properties of Organic Molecules: Origin, Theory. CD, ORD – VCD- principles and applications, haloketone rules, sector rules, helicity rules.

D: Metallocenes, non benzenoid aromatics and polycyclic aromatic compounds,

Bonds weaker than covalent – addition compounds, crown ether, complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Course No. 303-A

A: Advanced Heterocyclic Chemistry – II

Indoles, pyrimidines, pyridazines, pyrazines, purines, pteridines compounds. Role of heterocyclic compounds in biological systems.

B: Organometallic Reagents

Principle, preparations, properties and application of organometallic compounds of transition elements – Cu, Pd, Ni, Fe, Co, Rh, Ru, Cr and Ti in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization), structure and mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction – Heck, Stille, Suzuki coupling, Sonogashia, Buchwald-Hartwig , Ziegler Natta reaction, Walker Process, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, functional organometallic compounds, pi-acid metal complexes, activation of small molecules by coordination.

C: Reagents in organic synthesis

Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, 1,3 - Dithane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Laweson's reagent. Wilkinson's catalyst, Baker yeast., hypervalent organo iodines (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

Course No. 304-A

Practical :

Organic multi-step preparations by the use of organic reagents and purification of the products by chromatographic techniques.

Extraction of Natural products & their purification (Thin layer and Column Chromatography) and partial characterization by IR, UV and NMR.

Semester – IV

Course No. 401-A

A: Spectroscopy – III

Application of DEPT, 1H- ^{1}H COSY, HETCOR, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, reaction monitoring etc. q - NMR & DOSY.

B: Bio-Organic Chemistry

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, Cyclodextrins, cyclodextrin-based models, calizazerenes, ionophores, micelles, synthetic enzymes or synzymes.

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structurecand Biological functions of coenzymes A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, EMN, FAD, lipoic, vitamin B_{12}. Mechanisms of reactions catalyzed by the above cofactors.

Course No. 402-A

A: Spectroscopy - IV

Modern techniques of mass spectroscopy: FAB, MIKE LCMS / MS, ES / MS, MS-MS.

B: Natural Products -III

Structure and Chemistry of quinoline alkaloids with special reference to cinchona group; isoquinoline alkaloids – morphine group.

Steroids: Occurrence, nomenclature, basic skeleton, and stereochemistry; Synthetic principles and chemical reactions.

Plant Pigments: Synthesis and reactions of Coumarin and Chromones; occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin Quercetin 3-glucoside, Vitexin, Diadzein, Butulin , Aureusin , Cyanidin-7-arabinoside, Cyanidin, Hirsutidin.

Biosynthesis of flavonolds: Acetate pathway and shikimic and pathway.

C: Green Chemistry

Green Chemistry – Overview, Set of Principles of Green Chemistry, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, solid phase organic synthesis.

Course No. 403-A

A: Nucleoside & Nucleotide

Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Replication, transcription, protein biosynthesis, Covalent interactions of nucleic acids with small molecules, Structural features of DNA and RNA.

B: Compounds of non metals

Chemistry of Organo sulphur, Organo phospohorus and organo silicon compounds.

C: Natural Products – IV

Structure, transformations, synthesis of simple and monoterpenoid derived indole alkaloids - reserpine, strychnine, ellipticine, lysergic acid.

Course No. 404-A

Practical :

Separation and identification of the components of a binary mixture of organic solids: chromatographic separation, purification and identification of individual components (use of IR, UV, NMR), derivatization of individual component and analytical establishment of their identity.

Multi-step organic preparations, Organoanalytical experiments / Project work.

Inorganic Chemistry

Semester-I

Course No. 102

A: Organometallic compounds of main group elements-**I**

Synthesis, properties and structures of organometallic compounds of group-I to group-III elements of the periodic table.

B: Clusters-**I**

Higher boranes, carboranes, metalloboranes and metallocarboranes.

C: Reaction mechanism of transition metal complexes-**I**

Classification of reactions of complex compounds, inert and labile complexes, consideration of octahedral substitution reactions in the light of VBT and CFT, energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ($\Delta S^{\#}$, $\Delta H^{\#}$, $\Delta V^{\#}$), substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc., conjugate base formation, anation reaction and base hydrolysis, reactions without metal-ligand cleavage.

D: Magnetic properties and spectra-**I**

Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, Russell-sander's terms, determination of magnetic susceptibility, magnetic properties of first transition series metal ions and lanthanides.

Course No. 104(Inorganic)

Practical :

Inorganic qualitative analysis: Less common metals – Be, Mo, W, Ti, Zr, Th, V, U, Ce and all the radicals included in the B. Sc (Honours) Chemistry syllabus.

Semester-II

Course No. 202

A: Organometallic compounds of main group elements-**II**

Synthesis, properties and structures of organometallic compounds of group-IV & V elements of the periodic table.

B: Reaction mechanism of transition metal complexes-**II**

Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter, etc.

Redox reactions- complementary and non-complementary reactions, mechanisms of outer sphere and inner sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross relation.

C: Clusters-**II**

Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds, isopoly and heteropoly acids and their salts.

D: Magnetic properties and spectra-**II**

CFT and its limitations, Orgel diagrams and spectra, calculations of Dq , B and β - parameters, charge transfer spectra, anomalous magnetic moment, magnetic exchange coupling and spin crossover.

Course No. 204(Inorganic)

Practical : Inorganic quantitative analysis:

Separation and estimation of two metal ions from minerals, alloys or solutions.

Semester-III

Course No. 301-B

A: Analytical Chemistry-**I**

Recapitulation of the elementary concepts of Analytical Chemistry.

Selected analytical techniques-**I**

Solvent extraction., High performance liquid chromatography (Brief ideas).
Ion exchange chromatography, Electro-analytical techniques.

B: Quantum chemistry

Many electron treatment, Pure-spin states, Slater-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothan method, Basic functions, Electron correlation, Configuration interaction, Born-Oppenheimer approximation, Introduction to Density function theory.

C: Characterization of inorganic compounds by vibrational, rotational spectroscopy, ESR, Mössbaur & EXAFS.

Course No. 302-B

A: Molecular symmetry and group theory

Symmetry elements and symmetry operations, definition of group, sub group, relation between orders of a finite group and its sub groups, conjugacy relation and classes, point symmetry group, Schonflies symbols, representation of groups by matrices, character of a representation, the great orthogonality theorem (without proof) and its importance, character tables and their use.

B: Solid state chemistry-**I**

Electronic properties and Band theory in relation to selected inorganic compopunds.

C: Chemistry of: i) Actinides. ii) Boranes and their related compounds.

D: Organotransition metal chemistry-**I**

Alkyls and aryls of transition metals.
Compounds of transition metal-carbon multiple bonds.
Transition metal- π -complexes.

Course No. 303-B

A: Chemical bonding-**I**

Crystal field theory- splitting of d- orbitals in electrostatic fields of different symmetry, 10Dq value, spectrochemical series, structural effects of CF splittings- ionic radii, Jahn Teller effects, thermodynamic effect of CF splitting- hydration, ligation and lattice energies, Irving-William series of formation constants, site preference in mixed metal oxides (Spinel and inverse spinel structures), defect of CFT, experimental evidence for metal-ligand overlap, MOT for bonding in complex compounds including σ - and π -bonding, comparison of VBT, CFT and MOT (Application of group theory as and when needed in the above cases).

B: Bio-inorganic Chemistry-**I**

Metal ions in biological systems, essential and trace elements,

Transport and storage of dioxygen : hemoglobin, myoglobin, hemerythrin and hemocyanine.

Electron transfer in biology:

Structure and functions of metalloproteins in electron transfer process: iron-sulfer proteins, cytochromes.

C: Photoinorganic Chemistry

Basics of photochemistry, properties of excited states, excited states of metal complexes, ligand field photochemistry, redox reactions by excited metal complexes, metal complex sensitizers, photo-splitting of water and solar energy conversion/storage.

Course No.304-B

Practical :

Preparation of inorganic compounds and their study by IR, electronic, Mössbaur, ESR spectra and magnetic susceptibility measurements, handling of air and moisture sensitive compounds involving vacuum lines.

Selection can be made from the following or any other compound as selected by the teacher concerned:

1. Sodium amide.
2. Synthesis and thermal analysis of group II metal oxalate hydrate, atomic absorption analysis of Mg and Ca.
3. Trialkoxyboranes- Preparation, IR and NMR spectra.
4. Dichlorophenylborane-synthesis in vacuum line.
5. Preparation of Tin (IV) iodide, Tin (IV) chloride and Tin (II) iodide.
6. Relative stability of Tin (IV) and Pb (IV): Preparation of ammonium hexachlorosttanate, ammonium hexachloroplumbate.
7. Hexa-bis (4-nitropheoxy) cyclotriphosphazene.

8. Synthesis of trichlorodiphenylantimony (V) hydrate.
9. Sodium tetrathionate.
10. Metal complexes of dimethyl sulphoxide- $CuCl_2$.2DMSO, $PdCl_2$.2DMSO, $RuCl_2$.4DMSO.
11. Synthesis of metal acetylacetonate: Magnetic moment, IR, NMR.
12. Bromination of $Cr(acac)_3$.
13. Magnetic moment of $Cu(acac)_2.H_2O$.
14. Cis and Trans $[Co(en)_2Cl_2]^+$.
15. Separation of optical isomer of cis-$[Co(en)_2Cl_2]Cl$.
16. Ion-exchange separation of oxidation state of vanadium.
17. Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), determination of O_2 absorption by Co(salen), reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
18. Preparation of Fe (II) chloride.
19. Preparation of Fe (II) chloride.
20. Reaction of Cr (III) with a multidentate ligand: a kinetics experiment (visible spectra Cr-EDTA complex).
21. Preparation of [Co(phenonthroline-5,6-quinone].
22. Preparation and use of Ferrocene.
23. Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
24. Preparation of phosphine and its transition metal complexes.
25. Any other experiment such as conversion of p-xylent to terephthalic acid catalysed by $CoBr_2$ (Homogeneous catalysis).
26. Preparation of tetraphenyltin.
27. Preparation of lithiated reagents.

Experiments will be set depending upon the availability of instruments and materials.

Semester-IV

Course No. 401-B

A: Analytical Chemistry-II

Selected analytical techniques-II

- Spectrophotometry.
- Thermal methods of analysis.
- Radioactive methods of analysis.
- Fluorimetry, nephelometry, turbidometry and atomic absorption spectroscopy.

B: Bio-inorganic Chemistry-II

Photosynthesis: PS-I & PS-II, nitrogenase, metal ion storage and transport, metalloenzymes, Na^+/K^+ pumps.

C: Molecular spectroscopy

Hamiltonian in presence of electric and magnetic field, interaction with electromagnetic radiation, induced emission and absorptions, the Einstein transition probabilities.

Electronic absorption spectroscopy- potential energy curves, Franck-Condon principle, oscillator strength, selection rules and intensity of electronic transitions, charge transfer spectra.

D: Organotransition metal chemistry-II

Transition metal compounds with bonds to hydrogen.

Organometalic catalysts.
Fluxional organometallic compounds.

Course No. 402-B

A: Characterization of inorganic compounds by NMR, ORD/CD & ESCA.

B: Chemical bonding-II

Charge transfer spectra, electron absorption spectra, d^1 and d^9 systems, multi-electron systems, Tanabe-Sugano diagrams for various d^n - configurations, ACFT.

C: Chemistry of non-transitional elements

Compounds with B-N bonds, P-N bonds and S-N bonds.

D: Chemistry of the missing elements

Course No. 403-B

A: Solid state chemistry-II

Solid state reactions, general principles ,Crystal defects and non-stoichiometry of inorganic compounds, colour centre, photographic process, phosphors.

B: Crystal morphology:

Important minerals and different types of silicates: structural and physical properties.

C: Chemistry of materials:

i) Glasses, ceramics, composites, liquid crystals, ionic conductors, molecular devices, thin films.

ii) Inorganic supramolecular chemistry: Basic terms and concepts, nature and types of supramolecular forces, self-assembly of metal atoms/coordination, metal-organic frameworks (MOFs).

iii) Nanomaterials: Fundamental physical and chemical principles, characterization, fabrication and applications.

Course No.404-B

Practical :

1) Quantitative analysis.

2)Techniques like ion exchange, chromatography, solvent extraction, spectrophotometry, flamephotometry, nephelometry etc

Physical Chemistry

Semester - I

Course No.103

A: Quantum Chemistry - I

Schrödinger equation, Basic postulates and theorems, Physical interpretation of wave function, stationary states, operator formation, atomic unit system, Heisenberg's equation of motion, Particle in a box problem, Finite barrier problem and tunneling, Linear harmonic oscillator, Ladder operators, Angular momentum problem, Rigid rotor, Hydrogen atom problem and its implications.

B: Classical Thermodynamics

Brief review of 1^{st}, 2^{nd} and 3^{rd} laws of thermodynamics, Nernst heat theorem and the third law of thermodynamics, calculation of entropy changes in chemical reactions. Mathematical and thermodynamic probability, Entropy and probability, the free energy of a mixture, Partial molal quantities, Analytical form of the chemical potential in ideal solutions, Chemical potential of a solute in a binary solution, Application of Gibbs Duhem equation, Nonideal solutions, concept of activity: experimental determination of activity coefficients of non electrolytes, Application of thermodynamics to micelles and microemulsion.

C: Chemical Kinetics – I

Potential energy surface: reaction coordinates and reaction paths, Transition state theory and thermodynamics, Reactions in solutions: enzyme catalysis and enzyme inhibition reactions, ionic reactions, oscillating reaction.
Fast reactions: Flow and stop-flow technique, Flash photolysis, Relaxation and Nuclear magnetic resonance techniques.

D: Macromolecules

Polymer definition, various types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics and mechanism of polymerization .Molecular mass, number and mass average molecular mass, molecular mass determination by various methods (osmometry, viscometry, diffusion and light scattering), sedimentation, chain configuration of macromolecules, and calculation of average dimensions of various chain structures, visco-elasticity.

E: Introduction to spectroscopy:

Introduction to basic principles (Fourier transform and computer averaging techniques LASERS), Rotational spectra, The rigid and non rigid rotor model, Selection rules, Symmetric top molecules: prolate, oblate, Spectral intensity, degeneracy of rotational energy levels and total relative population, Isotopic substitution.

Vibrational and rotation-vibrational spectra, Simple harmonic oscillator model, Selection rules, Fundamentals and overtones, Hot bands, Q, P, and R branches, Chemical analysis by IR techniques.

Electronic system of diatomic molecules, Raman spectroscopy: Rayleigh and Raman scattering: stokes and anti stokes lines, Rotational and vibrational Raman spectra, Applications of Raman spectroscopy.

Course No. 104(Physical)

Practical :

1. Studies on the kinetics of iodination of acetone.
2. Determination of solubility product of PbI_2 by titrametric method.
3. Determination of coordination number of Cu^{++} (partition method).
4. Ion exchange capacity of resin.
5. Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.
6. Conductometric titration of a mixture of acids.
7. Estimation of acid potentiometrically.
8. Estimation of acid pH metrically.

Semester- II

Course No. 203

A: Quantum Chemistry - II

The variational method, Eckart's theorem, Linear variational method, Perturbation theory (time independent), Application of variational method and nondegenerate perturbation theory to the helium atom problem.

Electron spin, Antisymmetry principle, Spectroscopic term symbols, Spin-orbit coupling, Degenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect, Stark effect. Hückel M.O. theory for conjugated systems, bond order and charge density calculations, Introduction to the method of self consistent Field, Hartree method, Koopman's theorem.

B: Molecular Symmetry and Group theory

Symmetry elements and symmetry operations, Group theory: definitions and theories, multiple symmetry operations, multiplication table, molecular point groups, Simple ideas of representation and character table.

C: Computers for Chemists

Fundamentals of Computers, Elements of the computer language (FORTRON, BASIC, C), Constants and variables, Operations and symbols, Expressions, Arithmatic assignment statement, Input and Output format statement, Termination statements, Branching statements. Branching statements such as IF or GO TO statements of LOGICAL variables, Double precision variables. Subscripted variables and DIMENSION DO statement FUNCTION and SUBROUTINE COMMON and DO Statement FUNCTION and SUBROUTINE COMMON and DATA statements (above language features refer to FORTRON; may be changed appropriately for C / BASIC)

Development of small computer codes involving simple formulae in chemistry, such as equations for kinetics, radioactive decay etc, Evaluation of lattice energy and ionic radii from experimental data, Linear simultaneous equations to solve secular equations within the Hijckel theory. Elementary structural features such as broad lengths, bond angles, dihedral angles etc. of molecules extracted form a database such as Cambridge than base.

D: Electrochemistry

Ion-association, Formation of ion-pairs, triplets etc; Ion-solvent interactions, The Born model, structural treatment of ion-solvent interactions, ion-quadruple theory of solvation, The solvation number, Debye-Hückel theory, Debye-Hückel-Onsagar theory, Electrophoretic and relaxation effects, Wein effects, Debye – Fulkenhegen effect.

E: Molecular Spectroscopy

Time dependent perturbation theory: Harmonic – perturbation and Fermi golden rule, Einstein's coefficients of induced emission and absorption, molecular term symbols, Electronic spectra of polyatomic molecules. $n \rightarrow \pi^*$, $\pi \rightarrow \pi^*$, CT transition , Effect of solvent, Vibronic progression, Oscillator strength, Luminescence and energy transfer processes, Mössbauer Spectroscopy, Photoelectron spectroscopy, Theory and applications to magnetic resonance spectroscopy (NMR, ESR etc).

Course No. 204(Physical)

Practical :

1. Studies on alkalis hydrolysis of ethyl acetate conductometrically.
2. Determination of pK_1 and pK_2 of phosphoric acid potentiometrically.
3. Determination of pK_1 and pK_2 of phosphoric acid pH metrically.
4. Verification of Debye Hückel Onsager-equation.
5. Studies on the kinetics of reaction between $K_2S_2O_8$ and KI spectrophoto-metrically.
6. Studies on the kinetics of reaction between KBr_3 and KBr titrimetrically.
7. Potentiometric estimation of Fe (II) using $K_2Cr_2O_7$.
8. Ternary phase diagram of $H_2O/C_6H_6/CH_2COOH$.

Semester- III

Course No. 301-C

A: Advanced Quantum Chemistry

Many electron treatment, Pure-spin states, Slater-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method, Basis functions, Electron correlation, Configuration interaction, Born-Oppenheimer approximation, Introduction to Density functional theory.

B: Group theoretical representation and spectroscopy

Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems, Projection operator, Direct product representation. Applications: SALC, Spectroscope selection rules, Polyatomic vibration and normal modes.

Course No. 302-C

A: X-ray diffraction and Solid State

Bragg-Miller indices, X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Defects in solids: point, line and plane defects, Determination of equilibrium concentration of Scottky and Frenkel defects, F-centres/color-centres in ionic crystals, Band theory of solids, Semiconductors (extrinsic and intrinsic), hopping semi-conductors, rectifiers, transitors, Super conductivity, Oraganic conducting solids, solid state reactions.

B: Biophysical Chemistry

Structure of Biomolecules: protein, nucleic acid, carbohydrates and lipids, Membrane structure, Biomolecular complexes : protein-ligand, enzyme- substrate and drug-DNA complexes with examples. Techniques for study of biomolecular structure and function: Fluorescence and CD, surface tension, surface pressure area, etc measurements.

Course No. 303-C

A: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undermined multipliers). Partition functions-translational, rotational vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions, Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions.

B: Surface Chemistry

Surface tension, curved surfaces, Young-Laplace and Kelvin equations. Adsorption on solids, micelles reverse micelles, microemulsion, Thermodynamics of micellization, Application of micelles and microemulsion.

Course No. 304-C

Practical :

1. Determination of CMC and micellization parameters of an ionic surfactant conductometrically.
2. Studies on the effect of ionic strength on the micellization of SDS.
3. Spectral studies on Py - I_2 charge transfer complex.
4. Determination of the activation energy of the reaction between $K_2S_2O_8$ and KI.
5. Determination of the activation energy of the reaction between $KBrO_3$ and KBr.
6. Determination of isoelectric point of gelation viscometrically
7. Determination of E^o of Ag^+ /Ag electrole and solubility product of AgCl.
8. Estimation of Cl^-, Br^- and I^- in a mixture potentiometrically.

9. Determination of coordination number of Ag^{+} ion in Ag-ammine complex potentiometrically.
10. Determination of composition of Fe^{2+}- salicylate complex by Job's method.

Semester- IV

Course No. 401-C

A: Polymer Chemistry

Plastics, elastomers and fibers, Compounding, Processing techniques; models of polymers; viscoelastricity, Theory of polymers solutions, entropy and Flory-Huggins theory, Commercial polymer and bio-medical applications, Polyethylene, polyvinul chloride, polyamides, polyester, phenolic resins epoxy resins and silcone polymers, Functional polymers-Fire retarding polymers and electrically conducting polymers, Biomedical polymers-contact lens, dental polymers, artificial heart kidney, skin and blood cells, Organic and Inorganic polymers.

B: Advanced Electrochemistry

Structure of electrified interfaces, Guoy-Chapman, Stern, Tobin etc. models; overpotential, exchange current density, bulter volmer equation, Tafel plot.
Quantum aspect of charge transfer at the electrode – solution interfaces, Electrocapillarity (EC), nature of EC curves, Lipmann equation, Electrical double layer theory. Electrochemistry at semiconductor interfaces; Electrocatalysis, Photoelectrochemistry, Theory and application of polarography, cyclic-voltammetry.Bioelectrochemistry; Introduction to corrosion, forms of corrosion, corrosion monitoring and prevention methods.

Course No. 402-C

A: Chemical Kinetics

Theories of unimolecular reactions: Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK) and Rice-Ramsperger- Kassel-Marcus (RRKM) theories.

B: Non equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamicc for biological systems.

Course No. 403-C

A: Advanced Material

Glasses, ceramics, composites and Nano materials. Glasy state, glass formers and modifiers, applications, ceramic structures, mechanical properties, clay products, refractories, characterization, property and application. Preparation, characterization, properties, applications of nanomaterials.

Thin Films and Langmuir – Blagett films: Preparator techniques, chemical, MOCVD, sol-gel etc. CB films, growth technique, Properties and applications. Liquid Crystals: Mesomorphic behavior, different phases in liquid crystals order parameters, textures, twisted and chiral nematics, chiral nematics, application of liquid crystals.

B: Quantum statistical thermodynamics and nonequilibrium Statistical Mechanics:

Fermi-Dirac statistics, distribution law and applications to metal, Bose Einstein statistics-distribution law and application to helium. Elementary ideas of Brownian motion, Einstein theory, relation between diffusion and mobility, Langevin equition.

Course No. 404-C

Practical :

1. Determination of pK_a of methyl red indicator spectrophotometrically.
2. Determination of pK_a of phenolphthalein indicator spectrophotometrically.
3. Study the effect of ionic strength on the kinetics of $K_2S_2O_8$ + KI reaction.
4. Study on the effect of ionic strength on the kinetics of $KBrO_3$ + KBr reaction.
5. Study the kinetics of inversion of cane sugar polarimetrically.
6. Tensiometric study on the micellization of a nonionic surfactant.
7. Experiments on: Computer application in solving different physicochemical problems.

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