PROPOSED SYLLABUS FOR M.Sc. CHEMISTRY

SEMESTER-I

(THEORY & PRACTICAL)

CHOICE BASED CREDIT SYSTEM (C.B.C.S)

(2020-21)

The Syllabus and credits assigned is hereby approved.

DEPARTMENT OF CHEMISTRY

FACULTY OF SCIENCE

UNIVERSITY OF ALLAHABAD

PRAYAGRAJ – 211 002

M.Sc. CHEMISTRY

SEMESTER I - THEORY PAPER

CORE COURSE CODE - CHE 501 – INORGANIC CHEMISTRY

PAPER – I **Course Credit = 04**
(40 Lectures)

UNIT – I

Metal – Ligand Bonding in Transition Metal Complexes
Crystal field splitting diagrams in complexes and Jahn-teller distortion.

UNIT - II

Molecular orbital theory and its applications to metal complexes.

UNIT – III

Molecular Symmetry and Character Tables
Symmetry elements and symmetry operations, symmetry groups, Defining properties of a group, character tables and its application.

UNIT - IV

Symmetry in inorganic molecules, Symmetry consideration in simple inorganic and coordination compounds.

Reference Books:

1. Principles of Inorganic Chemistry by Puri, Sharma and Kalia
2. Inorganic Chemistry By Miessler and Tarr
3. Coordination Chemistry By Ajai Kumar
4. Spectroscopy Of Inorganic Compounds by J.D.Singh
5. Selected Topics in Inorganic Chemistry by Wahid , Tuli, Madan
6. Inorganic Chemistry by Alan G. Sharpe
7. Group theory and its applications by P.K.Bhattacharya
8. Group theory in Chemistry by M.S. Gopinathan and V.Ramakrishan
9. Symmetry and group theory in chemistry by R.Ameta
10. Group theory and spectroscopy by Alka L. Gupta
11. Chemical Applications of Group Theory by F.A.Cotton

SEMESTER – I PRACTICALS – LAB COURSE CODE CHE 533 INORGANIC CHEMISTRY (in addition to Core Course Code CHE 501)

Course Credit = 02 (40 hrs)

Qualitative Analysis

Qualitative mixture analysis for seven radicals including two rare elements. (Mo, W, Ti, Zr, Th, Ce, V) in cationic and anionic forms.

Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods

(i) Ni^{2+} (gravimetrically) and Cu^{2+} (Volumetrically)
(ii) Ba^{2+} (gravimetrically) and Cu^{2+} (Volumetrically)
(iii) Fe^{3+} (gravimetrically) and Ca^{2+} (Volumetrically)
(iv) Mg^{2+} (gravimetrically) and Ca^{2+} (Volumetrically)

SEMESTER I - THEORY PAPER

CORE COURSE CODE: CHE 502 –ORGANIC CHEMISTRY

PAPER – II

Course Credit = 04 (40 Lectures)

UNIT – I

Aromaticity and π-Molecular Orbitals of Conjugated Systems

Aromaticity in benzenoid, non-benzenoid compounds and metallocenes, Huckels rule, energy of pi-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity.

Reaction Mechanism: Structure and Reactivity

Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, Product analysis, Kinetic and stereochemical studies.

UNIT – II

Stereochemistry

Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, optical purity, enantiotopic and diasterotopic atoms, group and faces, stereospecific and stereoslective synthesis. Optical activity in the absence of chiral carbon (biphenyls allenes and spiranes), chirality due to helical shape, R/S Nomenclature, chiral centres and shiral molecules.

UNIT – III

Conformational Analysis

Factors responsible for the stability of conformation, Torsional strain, steric strain, Dipole-dipole interaction, Hydrogen bonding, angle strain, hyperconjugation, and anomeric effect. Conformation of CH_2OH-CH_2OH, 2-chloroethanol, haloalkanes, 1,2-difluoroethane, confirmation of cyclohexanone-$A^{1,2}$strain, cyclohexene and Confirmation of alkylidenecyclohexane- $A^{1,3}$ strain. Conformational analysis of cycloalkanes- disubstituted cyclohexanes, decalins. Effect of conformation on reactivity.

UNIT – IV

Aliphatic Nucleophilic Substitution

The S_N2, S_NI, mixed S_N1^1, S_N2^1, S_Ni and SET mechanisms, The neighboring group mechanism, neighboring group participation by P and S bonds, anchimeric assistance. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile and regioselectivity.

UNIT – V

Reaction intermediate

Generation, structure, stability and reactivity of nucleophilic carbenes, carbanion (enolate ion), non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangement

Aromatic Nucleophilic Substitution

The S_NAr, S_NI benzyne and $S_{RN}I$ mechanisms, Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

Reference Books:

1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. Peter Sykes, A Guide book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. M.S. Singh, Reactive Intermediates in Organic Chemistry, Structure, Mechanism, and Reactions, 2014 Wiley-VCH Verlag GmbH & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany.
4. Advanced Organic Chemistry (Reaction, Mechanism and Structure) by Jerry March
5. Stereochemistry: Conformation and Mechanism by P.S. Kalsi
6. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, Wiley Interscience, New York (2004).

SEMESTER – I

PRACTICALS -LAB COURSE

ORGANIC CHEMISTRY (in addition to Core Course Code CHE 502)

LAB COURSE CODE CHE 534

Course Credit = 02 (40 hrs)

(a) Separation and identification of organic compounds using chemical methods from binary mixtures.

(b) Estimation of glucose, aldehydes and ketones by chemical and spectroscopic methods.

SEMESTER I - THEORY PAPER

COURSE CODE: CHE 503 – PHYSICAL CHEMISTRY

PAPER – III

Course Credit = 04 (40 Lectures)

UNIT – I

Nernst Heat Theorem and its application to non-condensed systems, Statement of the Third Law of Thermodynamics, Relationship between entropy constant and Nernst chemical constant, Determination of entropy from the Third Law using the correction due to gas imperfections.

UNIT – II

Maxwell-Boltzmann statistics, partition function, Translational, rotational, vibrational, nuclear and electronic partition functions, Internal energy and heat capacity in terms of partition function.

UNIT – III

Rigid and non-rigid rotational spectra, selection rule, Isotopic shift, Rotational constant, Simple harmonic oscillator Experimental techniques, principle of vibration-rotation spectra, selection rule, PQR branches.

UNIT – IV

Step polymerization, Kinetics of step polymerization, Molecular weight averages, Method of determining the molecular weight by osmotic pressure and Light scattering.

Recference Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
4. Advanced Physical Chemistry by Gurdeep Raj

SEMESTER – I PRACTICALS – LAB COURSE

PHYSICAL CHEMISTRY

LAB COURSE CODE CHE 535

Course Credit = 02(40 hrs)

1. Kinetics of oxidation of reducing sugars by potassium ferricyanide or Copper (II) in presence of ammonium hydroxide or sodium hydroxide.

2. Kinetics of oxidation of alcohols or diols by aqueous alkaline hexacyanoferrate (III) ions.

3. Potentiometric titration of strong acid and strong base.

SEMESTER I - THEORY PAPER

CORE COURSE CODE: CHE 504 – ANALYTICAL CHEMISTRY

PAPER – IV

Course Credit = 04
(40 Lectures)

UNIT – I

Fundamentals of Chemical Analysis
Qualitative and Quantitative Analysis, Sensitivity and Selectivity of Analytical Methods, Sampling; Hydrogen ion exponent: Buffer solutions, Pseudo buffers, Standard Buffers: Problems based on acid-base, solubility and complex ion equilibria.

UNIT – II

Data Handling in Analytical Chemistry
Accuracy and Precision; Determinate and Indeterminate errors; Significant figures, Rounding off figures; Standard deviation; Propagation of errors. Regression analysis; Statistics of sampling and detection limit evaluation.

UNIT – III

Volumetric methods of analysis

Expressions of concentration of solutions: Molarity, Formality, Normality; Analytical and Equilibrium concentrations; Common Units for Expressing Trace Concentrations; Standard solutions; Volumetric calculations; Acid-base, redox, precipitation, complexometric and chelatometric titrations; Theory of Indicators – Mixed Indicators and Fluorescent Indicators.

UNIT – IV

Gravimetric Methods of Analysis

Weight relationships; Principles and scope of gravimetric methods; Conditions of Impurities in precipitates – Coprecipitation and post precipitation; Washing, filtering and drying of precipitates; Role of organic precipitants in gravimetric analysis, important organic precipitants: Dimethyl glyoxime, cupferron, 8-Hydroxyquinoline, salicyldoxime, 1-nitroso 2-napthol, Anthranic acid, α-benzoinoxime (Cupron), Sodium tetraphenylboron.

UNIT – V

Spot tests

Spot tests for metal ions –

Spot tests for identification of functional groups – hydroxy, carboxylic, nitro, nitroso, azo and amino.

Determination of elements and functional groups in organic compounds

Semimicro determination of carbon, hydrogen, sulphur and nitrogen.

Recference Books:

1. Quantitavive analysis by Vogels
2. Spectroscopy by B.K. Sharma

SEMESTER – I PRACTICALS – LAB COURSE
ANALYTICAL CHEMISTRY (in addition to Core Course Code CHE 504)

LAB COURSE CODE CHE 536

Course Credit = 02
(40 hrs)

1. Determination of replaceable hydrogen in Acid by titration with sodium hydroxide
2. Determination of Bicarbonate
3. Determination of water hardness with EDTA
4. Determination of Silver by Volhard's method
5. Determination of Chloride by Fajan's method
6. Analysis of Commercial hypochlorite or peroxide solution by iodometric titration

PROPOSED SYLLABUS FOR M.Sc. CHEMISTRY

SEMESTER-II

(THEORY & PRACTICAL)

CHOICE BASED CREDIT SYSTEM (C.B.C.S)

(2020-21)

The Syllabus and credits assigned is hereby approved.

DEPARTMENT OF CHEMISTRY

FACULTY OF SCIENCE

UNIVERSITY OF ALLAHABAD

PRAYAGRAJ – 211 002

M.Sc. CHEMISTRY

SEMESTER II - THEORY PAPER

CORE COURSE CODE - CHE 505 – INORGANIC CHEMISTRY

Course Credit = 04
(40 Lectures)

PAPER – I

UNIT-I

Reaction Mechanism of Transition Metal Complexes

Inert and labile complexes, Mechanism of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct indirect evidence in favor of conjugate mechanism.

UNIT-II

Anation reactions, reactions without metal ligand bond cleavage, Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction.

UNIT-III

Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

UNIT-IV

Term Symbols and Basic Principles of Electronic Spectroscopy

Frank – Condon principle, spin and Laporte selection rules, band intensities, band-width. Number of microstates and term symbols for gaseous atoms/ions. Spin-orbit coupling in spectroscopic ground state of p^2 and d^2 configurations and energies of J levels.

Reference Books:

1. Advanced Inorganic Chemistry By Ajai Kumar
2. Inorganic Chemistry by Shriver and Atkins
3. Inorganic Chemistry By Miessler and Tarr
4. Inorganic Reaction Mechanism by Indrajit Kumar
5. Spectroscopy of inorganic compounds by J.Singh, M.D.Pandey and Jaya Singh
6. Physical Methods in inorganic chemistry by Russel S. Drago
7. Theoretical Inorganic Chemistry by M.C.Dey and J. Selbin

SEMESTER – II PRACTICAL – LAB COURSE

INORGANIC CHEMISTRY (in addition to Core Course Code CHE 505)

LAB COURSE CODE-CHE 537

Course Credit = 02
(40 hrs)

Preparation of Coordination Complexes and their Characterization by m.p, elemental Analysis and molar conductivity measurements.

(a) $VO(acac)_2$
(b) $K_3[Cr(C_2O_4)_3].\ 3H_2O$
(c) $Na[Cr(NH_3)_2\ (SCN)_4]$
(d) $Mn(acac)_3$
(e) $K_3[Fe(C_2O_4)_3]$
(f) $Hg[Co(SCN)_4]$
(g) $[Co(Py)_2Cl_2]$
(h) $[Ni(NH)_6]Cl_2$

Study of recorded UV-visible and IR of above prepared coordination compounds

SEMESTER II - THEORY PAPER

CORE COURSE CODE: CHE 506 – ORGANIC CHEMISTRY

PAPER – II

Course Credit = 04 (40 Lectures)

UNIT-I

Free Radical Reactions

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes, Free radical rearrangement, Hunsdiecker reaction.

Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspect of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation, Stereochemistry of epoxidation and halo-lactonisation.

UNIT-II

Addition to Carbon-Hetero Atom Multiple Bonds

Generation of enolate ions and their synthetic applications. Stereochemistry of Wittig reaction and Aldol condensation. Stobbe condensation reactions. Hydrolysis of esters.

Elimination Reactions

The E_2, E_1 and E_1cB mechanisms and their stereochemistry and orientation. Reactivity-effects of substrates, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination and Peterson elimination.

UNIT-III

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1,3,5- hexatriene and allyl system, Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

UNIT-IV

Cycloadditions-antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolor cycloadditions and cheleoptropic rections.

UNIT-V

Sigmatropic rearrangement

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements, detailed treatment of Claisen and Cope-rearrangements. Fluxional tautomerism, Aza-Cope rearrangements. Introduction to Ene reactions. Simple problems on pericyclic reactions.

Reference Books:

1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. R.O.C. Norman and C. M. Coxon, Principles of Organic Synthesis, CRC Press, New York, 2009.
3. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
4. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition 1990), Macmillan India Ltd., New Delhi.
5. S.M. Mukherjee and S.P. Singh, Pericyclic Reactions, MacMillan India, New Delhi.
6. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic Reactions, Pragati Prakashan, 2005.
7. I. Fleming, Pericyclic Reactions, Oxford University Press, Oxford (1999).

SEMESTER – II

PRACTICAL – LAB COURSE

ORGANIC CHEMISTRY (in addition to Core Course Code – 506)

LAB COURSE CODE-CHE 538

Course Credit = 02 (40 hrs)

(a) Preparation of various organic compounds involving two or three steps employing different reactions viz. Aldol Condensation, reactions of enolate ions, oxidation reactions, Cannizzarro reaction, Molecular rearrangement reactions etc. with a view to give the student sufficient synthetic training in synthetic organic chemistry

(b) Isolation of:

a. Caffeine from tea leaves

b. Eugenol from cloves

SEMESTER II - THEORY PAPER

COURSE CODE: CHE 507 – PHYSICAL CHEMISTRY

Paper – III

Course Credit = 04 (40 Lectures)

UNIT-I

Postulates of quantum mechanics, three-dimensional time independent Schrodinger wave equation, Eigen functions and eigen values, one dimensional harmonic oscillator, Variation principle and its application to ground state H-atom.

UNIT-II

Thermodynamic formulation of rate constant, Comparison of collision and absolute rate theories, Calculation of transmission coefficient, Transition State Theory in Solution, Primary salt effect, The theory of Absolute reaction rates-for reactions between atoms and reactions between molecules in terms of partition function, Explosive reactions.

UNIT- III

Primary and secondary process in photochemistry, Photosensitization, Rice-Herzfeld mechanism, photochemical chain reactions (hydrogen chlorine, hydrogen bromine), non-chain photochemical reactions (formation of phosgene, decomposition oh H_2O in presence of CO)

UNIT-IV

Debye-Huckel Theory of the structure of dilute solution, Properties of ionic cloud, Limiting law and its verification, determination of partial molar volume. Crystal symmetry and miller indices, Brag's equation, X-ray analysis of NaCl.

Recommended Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
4. Advanced Physical Chemistry by Gurdeep Raj

SEMESTER – II PRACTICAL – LAB COURSE

PHYSICAL CHEMISTRY

LAB COURSE CODE -CHE 539

Course Credit = 02
(40 hrs)

1. Uncatalyzed oxidation of cyclic ketones by alkaline hexacyanoferrate (III).

2. Conductometric/Potentiometric titration of mixtures acids, KCL and KI.

2. Kinetics of oxidation of diols by cerium (IV) sulphate in aqueous sulphuric acid medium.

SEMESTER II - THEORY PAPER

COURSE CODE: CHE 508 – ANALYTICAL CHEMISTRY

PAPER – IV

Course Credit = 04
(40 Lectures)

UNIT-I

Ionic Equilibria in Solution

Activity and activity coefficients, Equilibrium constants in analysis and Systematic Approach to Equilibrium calculations – Mass Balance Equations and Charge Balance Equations; Numerical problems based on ionic equilibria.

UNIT-II

Potentiometry

Potentiometric Electrodes: Metal Electrodes, Metal – Metal Electrodes, Metal-Metal Salt Electrodes for measuring the Salt's Anion, Redox Electrodes, Reference Electrodes, Potentiometric titrations, Potentiometers and pH meter, Glass pH Electrode and its applications; Alkaline Error and Acid Error.

UNIT-III

Conductometric Methods

Principle of Analysis; Measurement of Conductance; Analytical Applications of Conductometry; Conductometric Titrations; High Frequency Titrations

UNIT-IV

Coulometry and Electrodeposition Methods

Electrolysis at Constant Potential, Electrolysis at Constant Current, Coulometric Methods of Analysis, Applications of Coulometry, Coulometric titrations and their applications.

UNIT-V

Spectrochemical Methods and Quantitative Aspects of Spectrochemical Methods

Interaction of Electromagnetic Radiation with Matter – Electromagnetic Spectrum, Mode of Absorption of Radiation by Matter, Rotational transitions, Vibrational transitions, Electronic transitions; Absorption by Isolated chromophores, Absorption by conjugated chromophores, Absorption by Aromatic compounds, Absorption due to chelate formation and metal complex formation.

Beer's law and its deviation and its applications, Mixture of absorbing species Spectrophotometric Instrumentation – Monochromators, Sample cells, Detectors, Types of Instruments-Single beam spectrophotometers and Double beam spectrophotometers, Spectrophotometric Error in Measurements.

Recference Books:

1. Analytical Chemistry by Gary D. Christian, Purnendu K. Dasgupta, Kevin, A.Schug, Willey publications.
2. Instrumental methods of Chemical analysis by H.Kaur, Pragati Prakashan, Merrut.

SEMESTER – II PRACTICAL – LAB COURSE

ANALYTICAL CHEMISTRY (in addition to Core Course Code CHE 508)

LAB COURSE CODE -CHE 540

Course Credit = 02
(40 hrs)

1. p*H* titration of unknown soda ash
2. Spectrophotometric determination of iron
3. Determination of nitrate in water by spectrophotometry
4. Spectrophotometric determination of manganese and chromium in mixture
5. Conductometric titration
6. Potentiometric titration

PROPOSED SYLLABUS FOR M.Sc. CHEMISTRY

SEMESTER-III

(THEORY & PRACTICAL)

CHOICE BASED CREDIT SYSTEM (C.B.C.S)

(2020-21)

The Syllabus and credits assigned is hereby approved.

DEPARTMENT OF CHEMISTRY

FACULTY OF SCIENCE

UNIVERSITY OF ALLAHABAD

PRAYAGRAJ – 211 002

M.Sc. CHEMISTRY

SEMESTER III - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 509

Course Credit = 04
(40 Lectures)

PAPER – I

Bioinorganic Chemistry (40 Lectures)

UNIT-I

Role of Metal Ions in Biological Systems
Photosystems; nitrogen fixation, Na^+ / K^+ pump.

UNIT-II

Complexes of Biological Significance
Metal complexes of porphyrins and phthalocyanin, Vitamin B_{12} and B_6; chloropyhylls.

UNIT-III

Metallo Proteins
Function, Electronic structure, bonding and stereochemistry of the active site – (1) Natural oxygen carring proteins – Haemoglobin, Myoglobin, Hemerythrins and Hemocyanin
(2) Electron Transport Protein – (a) Iron – sulfer Proteins – Rubredoxin and Ferrodoxins (b) Cytochromes (types a, b and c)

UNIT-IV

Metallo enzymes –
Mo-containing Enzymes – Nitrogenase; Xanthine Oxidase, sulphite, Oxidase and Nitrate reductase (b) Iron-containing Enzymes – cytochrome – c- oxidase, catalases, Peroxidases, cytochrome-p-450

Reference Books:

1. Bio-inorganic Chemistry by Asim k Das
2. Organometallic and Bioinorganic Chemistry by Ajai Kumar
3. Inorganic Chemistry by Shriver and Atkins
4. Elements of Bio-inorganic chemistry by G.N. Mukherjee and A. Das
5. Inorganic Chemistry-Principles of Structure and Reactivity by James Huheey , Ellen A. Keiter, R. L.Keiter and Okhil k. Medhi

M.Sc. CHEMISTRY

SEMESTER III - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 510

Course Credit = 04
(40 Lectures)

PAPER – II

Organometallic Chemistry

UNIT-I

Classification of organometallic compounds based on hapticity and polarity of M-C bond; Nomenclature and general characteristics.

UNIT-II

Complexes of σ-Donar π -donor Organic Ligands
Transition metal alkenyls, alkynyls, carbenes and carbines.
Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and arene complexes, important reactions with special reference to nucleophilic and electrophilic attack on ligands and to organic synthesis.

UNIT-III

Transition Metal Compounds in Homogeneous Catalysis and compounds with M-H bond - Hydrogenation, hydroformylation and Zeigler-Natta polymerization of olefins.

UNIT-IV

Waker Process, hydrocarbanylation of olefins, oxopalladation reactions, activation of C-H bond. Metal hydrides (classical and non-classical).

UNIT-V

Fluxional Organometallic Compounds
Fluxionalloy and dynamic equilibria in compounds such as n^2 – olefins and n^3 – allyl and dienyl complexes.

Reference Books:

1. Inorganic Chemistry-Principles of Structure and Reactivity by James Huheey
2. Inorganic Chemistry by Shriver and Atkins
3. Basic Organometallic Chemistry By Anil Elias
4. Organometallic and Bioinorganic Chemistry By Ajai Kumar
5. Inorganic Chemistry by Alan G. Sharpe

M.Sc. CHEMISTRY

SEMESTER III - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 511

Course Credit = 04
(40 Lectures)

PAPER – III
Coordination Polymers, Cages, Clusters and Nanostructures

UNIT-I

Coordination Polymers

Classification, types of metal-organic frameworks (MOFs), Synthetic strategies, charactization, properties and applications.

UNIT-II

Metal Carbonyls and related Compounds

Preparation structure and properties; bonding in metal carbonyls, variants of CO bridging vibrational spectra of metal carbonyls, principle reaction types of metal carbonyls, metal nitrosyl.

UNIT-III

Polyhedral Boranes

Higher boranes, carboranes, metallo-boranes and metallo-carboranes – Structure and bonding in the light of Wade's and Jemmis' Rules.

UNIT-IV

Synthesis and applications of nanoparticles

Introduction of Nano Particles; its different methods for preparation; its applications to chemistry.

Reference Books:

1. Concise Inorganic Chemistry by J.D. Lee
2. Principles of Inorganic Chemistry by Puri, Sharma and Kalia
3. Inorganic Chemistry by Purcell Keith
4. Basic Inorganic Chemistry by F. Albert Cotton , Geoffrey Wilkinson , Paul L. Gaus
5. Concepts and Models of Inorganic Chemistry by B.Douglas , D.Mc Daniel and J. Alexander
6. Fundamentals of Nanoparticles by Abdel Salam Hamdy Makhlouf, Ahmed Barhoum
7. ***Introduction to Nano Basics to Nanoscience and Nanotechnology*** by Amretashis Sengupta; Chandan Kumar Sarkar
8. ***Inorganic Chemistry by James E. House***

SEMESTER III - PRACTICALS CHEMISTRY

LAB COURSE CODE-INORGANIC CHE- 541

(In addition to CHE CODE- 509, 510 & 511)

Course Credit = 04
(40 Lectures)

Separation of a Mixture of Cations/Anions by Paper Chromatographic Technique Using Aqueous/Non-aqueous Media:

(i) Pb^{2+} and Ag^{+} (aqueous and non-aqueous media)

(ii) Co^{2+} and Cu^{2+} (non aqueous media)

(iii) Cl^{-} and I^{-} (aqueous – acetone media)

(iv) Br^{-} and I^{-} (aqueous – acetone media)

Ion-exchange Method of Separation

(i) Separation of Zn^{2+} and Mg^{2+} on an anion exchanger

(ii) Separation of Co^{2+} and Ni^{2+} on an anion exchanger

SEMESTER III - THEORY PAPER
(SPECIALIZATION IN ORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 512

Course Credit = 04 (40 Lectures)

PAPER – I: Rearrangements and Photochemistry

UNIT-I

Molecular Rearrangements

Migration to electron deficient carbon atom

Pinacole-Pinacolone rearrangement, Wagner-Meerwein rearrangement, Tiffeneau-Demjanov ring expansion, Dienone-Phenol rearrangement, Benzil Benzilic acid rearrangement, Favorski rearrangement.

UNIT-II

Migration to electron deficient nitrogen atom

Wolf, Hofmann, Curtius, Losen, Schmidt, Beckmann rearrangement.

Migration to electron deficient oxygen atom

Baeyer-Villiger rearrangement.

UNIT-III

Photochemistry of Carbonyl Compounds

Photochemistry of enones, hydrogen abstraction.

UNIT-IV

Rearrangements of α, ß - unsaturated ketones and cyclohexadienones, photochemistry of p-benzoquniones.

UNIT-V

Photochemistry of unsaturated system

Olefins, cis-trans isomerisation, dimerisation, hydrogen abstraction and additions. Acetylenes-dimerisation, Dienes-photochemistry of 1, 3-butadiene (2+2) additions leading to cage structures, photochemistry of cyclohexadienes, Photochemistry of aromatic compounds-exited state of benzene and its 1,2 and 1, 3-shifts, Photo-Fries rearrangement, Photo-Fries reaction of anilides, photosubstitution reaction of benzene derivatives, Photolysis of nitride esters and Barton reaction.

Reference Books:

1. Organic Synthesis by Prof. J. Singh & Prof. L.D.S. Yadav
2. Molecular Rearrangements in Organic Synthesis by Christian M. Rojas
3. H.O. House, Modern Synthetic Reactions, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.
4. L.F. Fieser and M. Fieser, Reagents for Organic Synthesis, Vol. 1-16 (Vol. 1, 1967), Wiley-Interscience, New York.
5. M. B. Smith, Organic Synthesis, McGraw Hill Inc., New York (1995).
6. P. R. Jenkins, Organometallic Reagents in Synthesis, Oxford science Publ., Oxford (1992).

SEMESTER III - THEORY PAPER
(SPECIALIZATION IN ORGANIC CHEMISTRY)
CORE COURSE CODE - CHE 513

Course Credit = 04 (40 Lectures)

PAPER - II: Oxidation, Reduction and Organometallic Reagents

UNIT-I

Oxidation

Hydrocarbons-alkenes, aromatic rings, saturated, C-H groups (activated and unactivated), alcohols, diols.

UNIT- II

Aldehydes, ketones and carboxylic acids, amines, hydrazines and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

UNIT-III

Reduction

Hydrocarbons –alkenes, alkynes and aromatic rings

Carbonyl Compounds: aldehydes, ketones, acids and their derivatives

Epoxides

Hydrogenolysis

UNIT-IV

Organometallic Reagents

Synthetic applications of organometallic compounds with mechanistic details of following metals. Hg, Cd, Ce, Cu, Ni, Fe, Co, Rh, Cr and Ti

UNIT- V

Application of Pd(o) and Pd(II) complexes in organic synthesis – Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

Reference Books:

1. Organic Synthesis by Prof. J. Singh & Prof. L.D.S. Yadav
2. Modern methods of organic synthesis by W. Carruthers

SEMESTER III - THEORY PAPER
(SPECIALIZATION IN ORGANIC CHEMISTRY)
CORE COURSE CODE - CHE 514

Course Credit = 04 (40 Lectures)

PAPER – III: Strategies in Organic Synthesis

UNIT-I

Disconnection Approach

General introduction to synthons and Synthetic equivalents, Disconnections, (C-C, C-S, C-O, bonds).

UNIT-II

Functional group interconversion, chemoselectivity, cyclisation reaction choosing synthetic route for small and large scale synthesis.

UNIT-III

Protecting Groups

Principle of protection of alcoholic, amino, carbonyl and carboxylic groups.

UNIT-IV

Stereochemistry in Organic Synthesis

Stereoselectivity and stereospecificity. Regioselectivity and regiospecificity: Assymmetric synthesis- Sharpless asymmetric epoxidation.

UNIT-V

Synthetic Strategies

(i). For formation of carbon-carbon bond.

(ii). For formation of carbon-nitrogen bond.

(iii). For formation of carbon-halogen bond.

(iv). For Ring Synthesis

(v). For Multistep Synthesis

Reference Books:

1. Organic Synthesis: The Disconnection Approach by Stuart Warren
2. Protecting Groups in Organic Synthesis by Peter G.M. Wuts
3. Protecting Groups in Organic Synthesis by James R. Honson
4. Sterochemistry of Organic Compounds by D. Nasipuri

SEMESTER III - PRACTICAL CHEMISTRY

LAB COURSE CODE-ORGANIC CHE- 542

(In addition to CHE CODE - 512, 513 & 514)

Course Credit = 02 (40 hrs)

(a) Separation and identification of organic compounds using chemical methods from organic mixtures containing up to three components

(b) Preparation of organic compounds involving several stages (c) Verification of Lambert Beer's Law using bromocresol green reagent. (d)Estimation of carbohydrates, protein, amino acids, ascorbic acid, blood cholesterol and aspirin in APC tablets by UV-Visible spectrophotometric method.

SEMESTER III - THEORY PAPER

(SPECIALIZATION IN PHYSICAL CHEMISTRY)

CORE COURSE CODE: CHE 515

PAPER – I

Course Credit = 04 (40 Lectures)

UNIT-I

Distribution law (Barometric formula), Sedimentation equilibrium, Maxwell's law of distribution of velocity and energy, R.M.S., Mean and Most probable velocities, Collision frequency, Collision between like and unlike molecules, Triple collision.

UNIT-II

Viscosity, Thermal conductivity and Diffusion coefficient of gases (quantitative treatment), Mean free path. Indistinguishability of gas molecules.

UNIT-III

Maxwell-Boltzmann law for gaseous system, Thermodynamic functions for gaseous systems, Molar heat capacity of gases, Heat capacity of hydrogen at low temperatures, Heat capacities of monoatomic crystals, The Einstein model, Debye's theory of solid.

UNIT-IV

Third law of thermodynamics (i) Nernst Heat Theorem (ii) Entropy of chemical reactions (iii) statements of third law of thermodynamics and (iv) Conventional entropies, Expression of equilibrium constant in terms of partition functions, Bose-Einstein statistics. Fermi Dirac Statistics, Comparison of M-B, B-E and F-D statistics.

Reference Books:

1. Physical Chemistry Book by P. C. Rakshit
2. Physical Chemistry by R L Madan
3. Physical Chemistry by Atkins'
4. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
5. Advanced Physical Chemistry by Gurdeep Raj

SEMESTER III - THEORY PAPER
(SPECIALIZATION IN PHYSICAL CHEMISTRY)
CORE COURSE CODE: CHE 516
PAPER – II

Course Credit = 04 (40 Lectures)

UNIT-I

Magnetic susceptibility and its determination, susceptibility equivalents, Diamagnetism of elements, Compounds and its ions, Langevin's theory of paramagnetism, Curie's law, Weiss molecular field theory of paramagnetism, Curie-Weiss law, Determination of Curie point.

UNIT-II

Bohr magneton, L-S and J-J couplings. Electronic spectra of molecules, Born-Oppenheimer approximation, Franck-Condon principle, Rotational fine structure of Electronic-Vibration transitions, Predissociation spectra.

UNIT-III

Quantum theory of Raman Spectra, Stokes and Antistokes lines, Rotation and vibration Raman spectra, Mutual exclusion principle, Theory of NMR relaxation process and chemical shift, The coupling constant, Nuclear spin interaction, Mossbauer spectroscopy and its principle, Origin of line width, Isomer shift, Quadropole effects, Application of Raman, NMR and Mossbauer spectra.

UNIT- IV

Overpotential, The current-potential relation, The Tafel equation, Hydrogen overvoltage and decomposition potential, Butler-Volmer equation, H_2-Evolution mechanism

Reference Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
4. Advanced Physical Chemistry by Gurdeep Raj
5. PHYSICAL CHEMISTRY: Volume-I&II by Ashish Kumar Nag.
6. Physical Chemistry Book by P. C. Rakshit

SEMESTER III - THEORY PAPER
(SPECIALIZATION IN IPHYSICAL CHEMISTRY)
CORE COURSE CODE: CHE 517
PAPER – III

Course Credit = 04 (40 Lectures)

UNIT-I

Kinetics of fast reactions, Techniques of study of fast reactions with reference to stopped flow, T-Jump and relaxation phenomena, Kinetics of oscillating reactions with special reference to Belousov-Zhabotinskii mechanism (B-Z mechanism).

UNIT- II

Thermodynamic functions for non-equilibrium states, Postulates and methodology, Linear laws, Gibbs equation, Entropy production and entropy flow, Phenomenological equations, Microscopic reversibility and Onsager's reciprocity relations.

UNIT-III

Nature of intermolecular forces, linear oscillating dipoles, Various contributions of intermolecular forces, London theory of dispersion forces, Partition functions for system of independent particles.

UNIT-IV

Partition function (pressure, free energy and fugacity) of imperfect gas, Generalized model of imperfect gas and L-J potential and evaluation of second virial coefficient.

Reference Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
4. Advanced Physical Chemistry by Gurdeep Raj
5. PHYSICAL CHEMISTRY: Volume-I&II by Ashish Kumar Nag.
6. Physical Chemistry Book by P. C. Rakshit.

SEMESTER III - PRACTICALS CHEMISTRY
LAB COURSE CODE-PHYSICAL CHE- 543
(In addition to CHE CODE - 515, 516 & 517)

Course Credit = 04
(40 Lectures)

1. Kinetics of Pd(II) catalysed oxidation of reducing sugars by N-bromoacetamide in acidic medium.

2. Kinetics of oxidation of ketones by Ce(IV) sulphate in acidic medium catalysed by Ir(III) chloride .

3. Conductometric titration of mixtures of acid and base.

SEMESTER III - ELECTIVE PAPER
ELECTIVE COURSE CODE – CHE 551

Course Credit = 04
(40 Lectures)

PAPER – IV

Solid – State and Nuclear Chemistry

UNIT-I

Nuclear Energy (i)
Energy release in fission chain reactions, controlled release of fission energy use of moderators; Nuclear reactors including breeder reactors.

UNIT-II

Nuclear Energy (ii)
Energy release in fusion reactions; Principle of atom and hydrogen bombs. Nuclear Fuels-Fuel cycle & Fuel reprocessing.

UNIT- III

Radiochemical Analysis
(i) Activation analysis
(ii) Radiometric and radio – release methods

UNIT-IV

(i) Solid – State Chemistry
Theory of metals free electron, valence bond and molecular orbital theories, conductors, insulators and Semiconductors. Superconductivity.

UNIT-V

(ii) Solid – State Chemistry
Alloys and intermetallic compounds. Hume-Rothery Lattice defects in ionic crystals – stoichiometric and non-stoichiometric defects.

Reference Books:

1. Principles of Physical Chemistry by Puri, Sharama & Pathania.
2. Fundamentals of Radiochemistry by D.D. Sood, A.V.R. Reddy, N. Ramamoorthy

SEMESTER III - ELECTIVE PAPER

ELECTIVE COURSE CODE – CHE 552

Course Credit = 04
(40 Lectures)

PAPER – IV

Spectroscopy of Organic Compounds

UNIT-I

Nuclear Magnetic Resonance Spectroscopy
PMR Spectroscopy chemical exchange, effect of deuteration, complex spin-spin interaction between two, three four and five nuclei (first order spectra).

UNIT-II

Virtual coupling, Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplication of complex spectra-nuclear magnetic double resonance, contract shift reagents, solvent effects. Fourier transform technique, Nuclear Overhauser Effect (NOE). Resonance of other nuclei: F and P. Structural problems based on PMR.

UNIT-III

Carbon-13 NMR Spectroscopy
General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. DEP, INEP,APT techniques.
Two dimension NMR spectroscopy: COSY, NOESY and INADEQUATE techniques. Structural problem based on ^{13}C NMR.

UNIT-IV

Mass Spectrometry
Introduction, ion production-EI, CI, FD and FAB, factors, affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, Mc-Lafferty rearrangement Nitrogen

rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect of their structure determination.

UNIT-V

Structural problems by joint application of UV, IR, NMR (^{1}H & ^{13}C) and mass spectroscopy.

Reference Books:

1. Elementary Organic Spectroscopy by Y.R. Sharma
2. Organic Spectroscopy Principles, Problems and their solutions by Dr. Jagdamba Singh & Dr. Jaya Singh

PROPOSED SYLLABUS FOR M.Sc. CHEMISTRY

SEMESTER-IV

(THEORY & PRACTICAL)

CHOICE BASED CREDIT SYSTEM (C.B.C.S)

(2020-21)

The Syllabus and credits assigned is hereby approved.

DEPARTMENT OF CHEMISTRY

FACULTY OF SCIENCE

UNIVERSITY OF ALLAHABAD

PRAYAGRAJ – 211 002

M.Sc. CHEMISTRY

SEMESTER IV - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 521

PAPER – I

Structural Methods in Inorganic Chemistry

Course Credit = 04
(40 Lectures)

UNIT- I

NMR Spectroscopy (i) Use of Chemical shifts and spin-spin couplings for structural determination;Double resonance, and Dynamic processes in NMR; Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in ^{13}CNMR; Use of Chemicals as NMR auxillary reagents (shift reagents and relaxation reagents); ^{1}H NMR of paramagnetic substances.

UNIT- II

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine Splitting (isotropic systems); the g value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Karamer's degeneracy); Electron-electron interactions, Anisotropic effects (the g value and the hyperfine couplings); Structural applications of transition metal complexes.

UNIT- III

Infrared and Raman Spectroscopy: Basic Principle, Fundamental modes, Factors affecting vibrational frequency, Applications of vibrational spectroscopy in investigating (i) symmetry and shapes of simple AB2, AB3 and AB4 molecules on the basis of spectral data, (ii) mode of bonding of ambidentate ligands (thiocyanate, nitrate, sulphate and ureas).

Reference Books:

1. Spectroscopy Of Inorganic Compounds by J.D.Singh
2. Analytical Chemistry by B.K. Sharma
3. Introduction to Spectroscopy by Donald L. Pavia
4. Instrumental Methods of Chemical Analysis by H.Kaur
5. Chemical applications of group theory by F.A.Cotton
6. Symmetry and spectroscopy of molecules by K.Veera Reddy

M.Sc. CHEMISTRY

SEMESTER IV - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 522

PAPER – II

Course Credit = 04
(40 Lectures)

Structural Methods in Inorganic Chemistry

UNIT- I

Magnetic Proterties

Magnetic behaviours, recent methods of magnetic susceptibility measurements, anomalous magnetic properties of transition metal complexes, spin crossover phenomena, magnetic properties of binuclear metal complexes involving metal-metal exchange interaction (Bleaney-Bower equation).

UNIT- II

X-ray Photo electron Spectroscopy and Related Techniques

Basic principles, spectral features and their applications to structural determination of inorganic molecules and metal complexes: X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES).

UNIT- III

X-Ray Spectroscopy: X-ray Absorption Fine Structure Spectroscopy (EXAFS and XANE) with synchrotron radiations techniques and X-ray fluorescence (XRF).

UNIT- IV

UV Visible Spectroscopy

Theory and its applications to metal complexes

Reference Books:

1.Magnetic Properties of transition metal Complexes by Lewis Carlin
2. Inorganic Chemistry by Huheey
3. Spectroscopy Of Inorganic Compounds by J.D.Singh
4. Analytical Chemistry by B.K. Sharma
5.Magnetic Properties of transition metal complexes by D K Chakraborty
6. Photoelectron Spectroscopy and Metal Complexes by Shekhar Srivastava

M.Sc. CHEMISTRY

SEMESTER IV - THEORY PAPER

(SPECIALIZATION IN INORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 523

PAPER – III

Course Credit = 04
(40 Lectures)

Selected Topics in Inorganic Chemistry

UNIT- I

Photochemistry of Transition Metal complexes
Photoreactions of inorganic complexes.

UNIT- II

Electrochemical Methods
Cyclic voltammetry.

UNIT-III

Differential pulse voltammetry, anodic stripping voltammetry, chronoamperometry, coulometry.

Reference Books:

1. Magnetic Properties of transition metal complexes by D K Chakraborty
2. Vogels Qualitative Inorganic Analysis by G.Svehla
3. Vogel's –A Textbook of Quantitative Chemical Analysis
4. Magnetism and Transition metal complexes by F.E.Mabbs and D.J.Machin

SEMESTER IV - CHEMISTRY PRACTICALS

LAB COURSE CODE INORGANIC CHE 545

(in addition to CHE 521, 522 & 523)

Course Credit = 02
(40 hrs)

1. Spectroscopic Determinations

(a) Mn/Cr/V in steel Sample.
(b) Ni/Mo/W/V/U/ by extractive spectrophotometric method.
(c) Fluoride/ nitrite / Phosphate.
(d) Iron – phenanthroline complex: Job's method.
(e) Zirconium – Alizarin Red-S complexes: Mole-ratio method.
(f) Copper-Ethylene diamine complexes: Slope-ratio method.
(g) Iron-thiocyanate complex-Ionophortic method

2. Atomic Absorption Spectroscopy

(a) Estimation of metal ions.

3. Project Work

SEMESTER IV - THEORY PAPER
(SPECIALIZATION IN ORGANIC CHEMISTRY)
CORE COURSE CODE – CHE 524

Course Credit = 04 (40 Lectures)

PAPER – I: Biosynthesis and Chemistry of Natural Products

UNIT- I

Bio-synthesis of Natural Products

(a) The acetate hypothesis, poly β-Ketoacids, Biosynthesis, Biogenesis Primary and Secondary reactions involved in biosynthesis. Biosynthesis of poly-ß-ketoacid.

(b) Isoprene rule, mevalonic acid from acetyl Co-enzyme A. Biosynthesis of mono, sesqui,di and triterpenes.

(c) Shikimic acid pathway for biosynthesis of aromatic ring.

(d) General biosynthesis of alkaloids.

UNIT- II

Terpenoids and Carotenoids

Classification, isoprene rule. Structure determination, stereochemistry, synthesis of the following representative molecules: citral, α terpenol, farnesol, santonin, abietic acid and ß-carotene, menthol. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- III

Alkaloids

General methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, Structure, stereochemistry and synthesis of the following : Ephedrine, (+) nicotine, quinine and morphine. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- IV

Steroids

Basic skeleton Diel's hyadrocarbon and stereochemistry, structure determination and synthesis of cholesterol, testosterone, estrone and progesterone. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- V

Prostaglandins

Occurrence, nomenclature, classification. Synthesis of PGE_2 and PGF_{2a}

Plant Pigments

General methods of structure determination, synthesis of Apigenin, Quercetin Cyanidin Hirsutin. Quercetin-3 glucoside, Diazein and cyanidine-7 glucoside. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

Reference Books:

1. K.W. Bentley, The Alkaloids, Vol. I., Interscience Publishers, New York (1957).
2. I. L. Finar, Organic Chemistry, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
3. W. Apsimon, Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York (Vol. 1, 1973).
4. J.S. Bindra and R. Bindra , Creativity in Organic Synthesis, Academic Press, NY (1975).
5. J.S. Bindra and R. Bindra, Prostaglandins Synthesis, Academic Press. Inc., New York, London (1977).
6. Jagdamba Singh, Sayed Masood Ali & Jaya Singh, Natural Products Chemistry, Pragati Prakashan.

SEMESTER IV - THEORY PAPER
(SPECIALIZATION IN ORGANIC CHEMISTRY)

CORE COURSE CODE – CHE 525

PAPER-II

Course Credit = 04

UNIT- I

(i). Diastereoselective, π- facial addition of nucleophilic to chiral carbonyl compounds: Crams model and Felkin-Ann model

(ii). Stereoselective synthesis, Asymmetric synthesis: the principle of asymmetric synthesis. Achiral substrate modified by chiral auxiliary Prelog's rule

UNIT- II

Asymmetric synthesis by the use of:

(i). Chiral substrate having prochiral unit

(ii). Chiral auxiliary

(iii). Chiral reagents

UNIT- III

Stereochemistry of some reaction:

(i). Mc-Marry reaction.

(ii). Corey-Winter reaction.

(iii). Fragmentation reaction.

(iv).Wittig and related reaction.

(v). Julia olefination.

UNIT- IV

Stereochemistry of some reaction :

(i). Conjugate addition with R_2CuLi

(ii). Mitsunobu reaction.

(iii). Stereochemistry of Pd catalyzed coupling reaction

(iv). Addition of Bromine and Peroxide on Cyclohexene.

UNIT- V

Vitamins: Structure determination including synthesis of Thiamine (Vitamin B1), Pyridoxine (Vitamin B6), Biotin (Vitamin H), Vitamin E

Reference Books:

1. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry of Natural Products by I. L. Finar
2. Modern methods of Organic Synthesis by W. Carruthers
3. Stereochemistry with applications to organic reactions by Prof. J. Singh, Prof. L.D.S. Yadav Dr. Jaya Singh & Dr. Santosh Singh
4. Organic chemistry by Clayden

SEMESTER IV - THEORY PAPER

(SPECIALIZATION IN ORGANIC CHEMISTRY)

CORE COURSE CODE - CHE 526

PAPER-III

Course Credit = 04 (40 Lectures)

Biomolecules

UNIT-I

Enzymes

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetic, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition, regulatory enzymes, Enzyme immobilization.

UNIT- II

Nucleic Acids

Secondary and Tertiary structure of DNA/RNA and stabilizing forces, polymorphic nature of DNA, Sequencing, solid phase synthesis; trimester, phosphoramidite and phosphonate methods, Purification : HPLC and gel electrophoresis. Peptide nucleic acid (PNA).

UNIT- III

Lipids

Chemistry and synthesis of phospholipids and glycolipids of lipid aggregates, micelles, bi-layers and biological membrane

UNIT- IV

Antibiotics

Synthesis of penicillin G, chloramphenicol, cephalosporin, tetracycline and streptomycin

UNIT- V

Pyrethroids and Rotenones, Pheromones

Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is

to be placed on the use of parameters wherever possible)

Reference Books:

1. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry of Natural Products by I. L. Finar
2. Lehninger Principles of Biochemistry by David L. Nelson & M.Cox

SEMESTER IV - CHEMISTRY PRACTICALS
LAB COURSE CODE ORGANIC CHE 546
(In addition to CHE 524, 525 & 526)

Course Credit = 02 (40 hrs)

(a) Estimation of $-NO_2$ group in organic compounds.

(b) Isolation of casein from milk, piperine from black papper and nicotine from tobacco.

(c) Applications of NMR spectrocopy (^{1}H & ^{13}C), UV, IR and Mass Spectroscopy in structure determination of organic and biologically important compounds

(d) Project

SEMESTER IV - THEORY PAPER
(SPECIALIZATION IN PHYSICAL CHEMISTRY)
CORE COURSE CODE: CHE 527
PAPER – I

Course Credit = 04 (40 Lectures)

UNIT- I

Ideal and non-ideal solutions, Inter-connection between Raoult's law and Henry's Law, Determination of Partial Molar Properties, Excess thermodynamic functions.

UNIT- II

Gibbs-Duhem-Margules equation and its applications, Activity and activity coefficients, Activity coefficients from excess thermodynamic functions, The theory of Van Laar, Scatchard Hildebrand theory.

UNIT- III

Huckel molecular orbital theory and its application to hybridization systems (ethylene, butadiene, allyls and benzene), Calculation of delocalization energy, Physical significance of charge density and bond order, Calculation of bond length, Pauling and Wheland's modification in HMO theory and it application to heteromolecules (pyrimidine).

UNIT- IV

Properties of colloids, sol-gel transformation, Colloidal electrolytes, Micellization and surfactants.

Reference Books:

1. A Textbook of Physical Chemistry by Mandeep Dalal
2. Physical Chemistry by R L Madan
3. Physical Chemistry by Atkins'
4. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
5. Advanced Physical Chemistry by Gurdeep Raj
6. PHYSICAL CHEMISTRY: Volume-I&II by Ashish Kumar Nag

SEMESTER IV - THEORY PAPER
(SPECIALIZATION IN PHYSICAL CHEMISTRY)
CORECOURSE CODE: CHE 528
PAPER – II

Course Credit = 04 (40 Lectures)

UNIT- I

Lattice energy of crystals, Cohesive energy, Free electron theory, Fermi-gas theory and band theory of solids, Metals, semi-conductors and insulators, Intrinsic extrinsic p-type and n-type semi-conductors,

UNIT- II

Internal pressure and its determination, Significance of internal pressure, Free volume of liquids and its determination, Application of free volume and its relation with energy and heat of vaporization.

UNIT- III

Partition function of a liquid, Outline of the theory of liquid state, Simple cell theory (Eyring equation) and cell model theory of Lennard-Jones and Devonshire, Eyring's free volume theory of liquid viscosity, Determination of partial molar volume and partial molar enthalpy,

UNIT- IV

Asymmetry and electrophoretic effects, Stoke's law and Walden product, Debye-Huckel-Onsager equation, Conductance ratio and the Onsager slope, Verification of Debye-Huckel-Onsager equation, Wien and Debye-Falkenhagen effects, Ion association in an electrolyte solution, Formation of pairs, triplets etc., Bjerrum theory of ion association.

Recference Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand
4. Advanced Physical Chemistry by Gurdeep Raj
5. PHYSICAL CHEMISTRY: Volume-I&II by Ashish Kumar Nag.
6. Principles of Physical Chemistry by B. R. Puri, Madan S. Pathania and L. R. Sharma.

SEMESTER IV - THEORY PAPER

(SPECIALIZATION IN PHYSICAL CHEMISTRY)

CORE COURSE CODE: CHE 529

PAPER – III

Course Credit = 04 (40 Lectures)

UNIT- I

Mechanism of Uni and bi-molecular surface reactions, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Absolute reaction rate theory of surface reactions.

UNIT- II

Comparison of homogeneous and heterogenous reactions, Study of equilibrium constant and steady state treatment for Arrhenius and Vant Hoff's complexes, Linear free energy relationship, Taft equation.

UNIT- III

Uncatalyzed and platinum group metals (osmium, ruthenium, iridium, rhodium etc.) catalyzed oxidation of organic compounds by $K_3[Fe(CN)_6]$ and Ce(IV) in alkaline / acidic medium.

UNIT- IV

Kinetic of initiation, retardation, Copolymerization (with special reference to monomer reactivates ratios), Coordination polymerization, Polyelectrolytes.

Reference Books:

1. Physical Chemistry by R L Madan
2. Physical Chemistry by Atkins'
3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand

4. Advanced Physical Chemistry by Gurdeep Raj
5. PHYSICAL CHEMISTRY: Volume-I&II by Ashish Kumar Nag

SEMESTER IV - CHEMISTRY PRACTICALS

LAB COURSE CODE PHYSICAL CHE 547

(in addition to CHE 527, 528 & 529)

Course Credit = 02
(40 hrs)

1. Study of cyclic alcohols by cerium (IV) sulphate in acidic medium in presence of iridium (III) chloride.
2. Ruthenium (III) chloride catalyzed oxidation of aliphatic or cyclic alcohols or glycols by alkaline hexacyanoferrate (III).
3. Kinetics of iridium (III) chloride catalyzed oxidation of aromatic aldehydes/alcohols/hydrocarbons by Ce(IV) sulphate in aqueous acidic medium.

SEMESTER IV - ELECTIVE PAPER

PAPER – I

ELECTIVE COURSE CODE – CHE 555

Course Credit = 04
(40 Lectures)

Enviornmental Chemistry

UNIT: I

Introduction to Enviornmental Chemistry
Concept and scope of environmental chemistry, Enviornmental terminology and nomenclatures, Environmental segments.

UNIT: II

The natural cycles of environment (Hydrological, oxygen, Nitrogen)

UNIT: III

Chemical Toxicology
Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

UNIT: IV

Air Pollution
Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, Photochemical smog, Air-quality standards.

UNIT: V

Water Pollution

Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and chlorine, chemical separation (Pb, As, Hg)

Reference Books:

1. Environmental Chemistry by A.K. De, New Age Publishers
2. Environmental Chemistry by P.S. Sindhu

SEMESTER IV - ELECTIVE PAPER

PAPER – II

ELECTIVE COURSE CODE – CHE 556

Course Credit = 04
(40 Lectures)

Reagents and Reactions

UNIT: I

Regents in Organic Synthesis

Use of following reagents in organic synthesis and function group transformation (including stereochemistry where possible)

Complex metal hydrides – $NaBH_4$, $LiAlH_4$, DIBAL, diborane, diisoamylborne, thexylborane, 9-BBN, isopinocamphenyl and diisopino-campherylborame, catechoborane
Gilman's reagent
Lithium disopropyl amide (LDA)

UNIT: II

Use of following reagents in organic synthesis and function group transformation (including stereochemistry where possible) :

Dicyclohexylcarbcarbodimide (DCC)
1, 3-Dithiane (Reactivity Umpolung)
Trimethylsily iodide
Tri n-butyltin hydride
DEAD

UNIT: III

Use of following regagents in organic synthesis and function group transformation (including stereochemistry where possible):

DDQ
Hydrazine and phenylhydrazine
Nucleophilic heterocyclic carbenes (NHC)
Nitrogen, Sulphur and Phosphorus Ylides
Preparation and their synthetic applications.

UNIT: IV

Selective Organic name reaction and their Synthetic Application

Stork Enamine reaction
Ene Reaction
Barton Reaction
Hofmann-Loffler-Freytag Reaction
Shapiro Reaction

UNIT: V

Green Chemistry

Introduction of green chemistry basic principles of green chemistry, organic synthesis using visible light, ionic liquid and PEGs.

Selective Organic name reaction and their Synthetic Application

Baylis-Hillman Reaction
Stetter Reaction

Reference Books:

1. Modern methods of organic synthesis by W. Carruthers
2. Organic Chemistry by Clayden
3. New trends in Green Chemistry by V.K. Ahluwaliya & M. Kidwai
4. Green Chemistry: An Introductory Text 2010 Edition by Mike Lancaster, Royal Society Of Chemistry