SEMESTER I - THEORY PAPER

CORE COURSE CODE: CHE 504 – ANALYTICAL CHEMISTRY

PAPER - IV

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.

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

SEMESTER II - THEORY PAPER

COURSE CODE: **CHE 508 – ANALYTICAL CHEMISTRY**

PAPER – IV

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.

SEMESTER – II PRACTICAL – LAB COURSE

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

LAB COURSE CODE AGR. CHE 540

Course Credit = 02
(40 hrs)

1. pH 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

SEMESTER III - THEORY PAPER

(Specialization in Analytical Chemistry)

CORE COURSE CODE – CHE 518

Course Credit = 04

PAPER – I
(Theoretical Aspects)

UNIT-I

Statistical Methods in Analytical Chemistry

(a) **Descriptive Statistics** : Distribution of random numbers, Gaussian distribution, other distributions, Central limiting theorem; Location parameters – Arithmetic, Geometric and Harmonic means, Median, Quartile; Confidence level and Confidence interval

(b) **Statistical Test**: Testing hypothesis-comparision of a mean with a true value : one –variable test, comparision of two means: two variable t – test; comparision of variables F-test, Testing for distribution x^2- test Test for outliers – Dixons -test

(c) Statistics of Sampling

UNIT-II

Liner least Squares : Least Squares plot; standard deviations of the slope and intercept; Correlation coefficient and coefficient of determination

UNIT-III

Graphic presentation of equilibrium data : acid base, solubility and complex formation

UNIT-IV

Kinetic Methods of Analysis : Enzyme catalysis – Enzyme kinetics, properties of enzymes, Enzyme Inhibitors and Activators; The Michaelis constant Determination of enzymes and Example of Enzymatic Analysis.

UNIT-V

Concept of Speciation – Iodine Species (I^-, IO^-_3, I_3^- and I_2); Actinide Speciation in Aquatic Environment, Lead, Chromium

SEMESTER III - THEORY PAPER

CORE COURSE CODE – CHE 519

Course Credit = 04
(40 Lectures)

PAPER - II
(Separation Techniques)

UNIT-I

Principles and applications of solvent extraction: quantitative treatments of extraction equilibria, solvent extraction of metals, analytical separation, multiple batch extraction, counter current distribution, synergistic extraction. Solid –phase extraction, Supramolecules in solvent extraction

UNIT-II

Ion exchange Resins – Mechanism of ion exchange, synthesis and characteristics of ion-exchange resins, Factors affecting the selectivity of ion exchange resin, Ion exchange capacity, Techniques in ion exchange methods and analytical applications.

UNIT-III

Ion Chromatography – Ion chromatography as a separation tool, Instrumentation in Ion chromatography; Analytical Applications of Ion chromatography

Adsorption chromatography:– Principle, Experimental Set up and use of Adsorption chromatography

UNIT-IV

Partition Chromatography- Principle of Liquid – Liquid partition chromatography Reversed Phase Partition chromatography, Application of Extraction Chromatography, Paper, Thin Layer and Ion-pair chromatography

UNIT-V

Electrophoresis – Principles of Electrophoresis – Classification of Electrophoresis Methods, Techniques of Electrophoresis and Instrumentation, Applications in Inorganic Chemistry, Separation of Biological Products.

SEMESTER III - THEORY PAPER

CORE COURSE CODE – CHE 520

Course Credit = 04
(40 Lectures)

PAPER - III
(Spectrochemical Methods)

UNIT-I

Turbidimetry and Nephelometry and their applications

Fluorometry – Principle of Fluorescence, Chemical Structures and Fluorescence, Relationship between concentration and Fluorescence Intensity, Fluorescence Irstrumentation

UNIT-II

Flame Emission Spectroscopy : Principles of Flame Photometry, Instrumentation Evaluation Methods in Flame Photometry

UNIT-III

Atomic Absorption Spectrophotometry (AAS) : Principles, Instrumentation, Interferences, Sample preparation, Applictions of AAS, Sensitivity and Detection Liimits in Analysis, Graphite Furnace in AAS

UNIT-IV

Inductively Coupled plasma Atomic Emission Spectroscopy : Limitation of Flame Emission spectroscopy, Principles of plasma spectroscopy, Inductively coupled Plasma Source, ICP-AES Instrumentation, Applications of Plasma Spectroscopy

UNIT-V

Principles of Infrared Spectrophotometry and Raman Spectroscopy, FT-IR and FT Raman Spectrometers, Applications of these techniques in Quantitative analysis.

SEMESTER III - PRACTICALS CHEMISTRY

LAB COURSE CODE-ANALYTICAL CHEM- 561

(In addition to CHEM CODE-526, 527 & 528)

Course Credit = 04
(40 Lectures)

1. Separation of Zn^{2+} + Mg^{2+} present in a sample using anion exchange resin and estimation of each metal ion thus separated by E.D.T.A. titration.

2. Separation of Co^{2+} + Ni^{2+} present in a sample using anion exchange resin and estimation of each metal ion thus separated by E.D.T.A. titration.
3. Determination of the pH of Hair shampoos.

4. Determination of the pk value of weak organic acid by pH titration.

5. U.V. Spetrophotometric determination of Aspirin, Phenacetin and Caffeine in APC tablets using solvent extraction Determination of Fe(III) by chloride extraction in ether

6. Separation of amino acids using paper chromatography

7. Electrophoresis

8. Flame emission photometric determination of sodium

9. Infrared determination of a mixture of Xylene isomers / APC tablet

10. Thin – Layer chramatograpy, Separation of Amino acids.

11. Water analysis

SEMESTER IV - THEORY PAPER

(Specialization in Analytical Chemistry)

PAPER –I

CORE COURSE CODE - CHE 530

Course Credit = 04
(40 Lectures)

Electroanalytical Methods

UNIT- I

Voltametry : The voltametric cell, the carrent voltage curve, the step wise reduction or oxidation supporting electrolyte chemicals modified electrodes.

UNIT- II

Polalography: The dropping mercury electrode, concepts of half wave potential, residual current, maxima, the Ilkovic equation, Ac polarography, Rapid scan Polarography, Square wave polarography, Inorganic and organic Polarography.

UNIT- III

Anodic stripping voltametry, cyclic voltametry squarewave polarography, chronopotentiometry.

UNIT- IV

Chemical Sensors classification, sensitivity and limit of detection, potentio-metric sensors Ion selective Electrodes (ISEs), types of electrodes, selectivity and applications of ISEs., Gas sensors, voltametric sensors

UNIT- V

Biosensors – Definition, The enzyme electrode, biosensors based on Ion-Selective electrodes, amperometric enzyme electrodes, applications of enzyme electrodes; Biosensors based on plant and animal tissue.

SEMESTER IV - THEORY PAPER

PAPER –II

CORE COURSE CODE – CHE 531

Course Credit = 04
(40 Lectures)

Other Methods in Analytical Chemistry

UNIT- I

Thermal and calorimetric methods of Analysis : Thermogravimetric Analysis (TGA) – Principle, apparatus and applications; Differential Thermal analysis (DTA) – Principle and apparatus; Derivative thermogravimetry – principle and apparatus, Interpretation of TGA and DTA curves. Thermometric titrations; Differential scanning calorimetry (DSC) - Instrumentation and Applications

UNIT- II

X-ray Emission Spectrometry : X-ray processes, X-ray Fluorescence, X-ray fluorescence Spectrometer, Applications of X-ray emission spectrometry.

UNIT- III

Mass spectrometry : Principles, Basic idea of techniques and applications

Gas chromatography and High Performance Liquid Chromatography : Principle, Instrumentation and Applications.

UNIT- IV

Polarimetry and Related methods: Polarised Light, Applications of Polarimatry, Optical Rotatory Dispersion (ORD) and Circular Dichromism (CD), Instrumentation for ORD and CD.

UNIT- V

The role of computers and microprocessors in Analytical Chemistry- Instrument optimizations, Data recording and storage, Data processing and data analysis (Chemometry), The scope of microprocessor Control and computers in analytical laboratories.

SEMESTER IV - THEORY PAPER

PAPER –III

CORE COURSE CODE – CHE 532

Course Credit = 04
(40 Lectures)

UNIT- I

Miscellaneous Analysis

Determination of moisture by Karl Fischer's method and active hydrogen by Zerwintinoff's method

UNIT- II

Gas Analysis – Volumetric methods of analysis of gases, determination to H_2O_2 (?), determination of available chlorine in bleaching powder.

UNIT- III

Analysis of oils and fats.
Acquaintance with commercial analysis of food materials like milk, butter, tea, sugar and vitamins.

UNIT- IV

Micro and Semi-micro determinations of functional groups like amino, nitro, azo, carbonyl, unsaturation, acetylenic hydrogen, sulphonic acid, sulphide, sulphamide and peroxides

UNIT- V

Micro and semi-micro determination of oxygen, phosphorus, arsenic and halogens (including fluorine in organic compounds).

SEMESTER IV - CHEMISTRY PRACTICALS

LAB COURSE CODE ANALYTICAL CHE 548
(in addition to CHE 530, 531 & 532)

1. Determination of calcium by Atomic Absorption spectrophotometry
2. Gas chromatographic analysis of a tertiary mixture
3. Enzymatic Determination of glucose
4. Determination of Cd^{2+} ion using polarography
5. Determination of Zn^{2+} ion using polarography
6. TGA
7. Least Square fitting
8. Composition of two sets of results of significance by

   (i) student's t-test (ii) F-test

Project Experiment

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

Moleculat Symmetry and Character Tables

Symmetry elememts 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.

UNIT - V

Molecular Luminescence

Principles of fluoresence and phosphorescence, Photolumionescence spectra of transition metal (d^{10}) and lanthanides complexes.

SEMESTER – I PRACTICALS – LAB COURSE

INORGANIC CHEMISTRY (in addition to Core Course Code CHE 501)

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 II - THEORY PAPER

CORE COURSE CODE - CHE 505 – INORGANIC CHEMISTRY

PAPER – I

Course Credit = 04
(40 Lectures)

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.

UNIT-V

Electronic Spectra of Transition Metal Complexes

Interpretation of electronic spectra using, Orgel and Tanabe – Sugano diagram for 3d transition metal complexes. Calculations of crystal field and ligand field parameters (Dq, B and ß parameters), nephelauxetic series and charge transfer spectra.

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 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

UNIT-V

Copper – containing Enzymes – Superoxide dismutase (SOD), Bovine Superoxide dismutase (BOD), ascorbic acid oxidase and (b) Zinc –

containg Enzymes carboxy – peptidase A and B; carbonic anhydrase and Urease.

SEMESTER III - THEORY PAPER

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.

SEMESTER III - THEORY PAPER

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.

UNIT-V

Alkoxides Properties; structural aspects of various types of alkoxides – Industrial applications and catalytic aspects of metal alkoxides.

SEMESTER III - PRACTICALS CHEMISTRY

LAB COURSE CODE-INORGANIC CHE- 541

Course Credit = 04
(40 Lectures)

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

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

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

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

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

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

Ion-exchange Method of Separation

e. Separation of Zn^{2+} and Mg^{2+} on an anion exchanger

f. Separation of Co^{2+} and Ni^{2+} on an anion exchanger

SEMESTER IV - THEORY PAPER

(Specialization in Inorganic Chemistry)

PAPER – I

CORE COURSE CODE - CHE 521

Course Credit = 04
(40 Lectures)

Structural Methods in Inorganic Chemistry

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

Nuclear Spectroscopy – (ii) Multinuclear NMR of Metal nuclei. ^{31}P, ^{9}F, ^{27}Al, ^{11}B, ^{119}Sn, $^{203/205}$Tl, ^{51}V etc.

UNIT- III

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- IV

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).

UNIT- V

Mass Spectrometry: Basic Principle, Fragmentation pattern and Fingerprint applications in the interpretation of Mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (ESI, TOF and FAB)

SEMESTER IV - THEORY PAPER

PAPER – II

CORE COURSE CODE - CHE 522

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

UNIT- V

Mossbauer Spectroscopy

Basic principle, conditions for Mossbauer spectroscopy, spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin – complexes, miscellaneous applications.
Nuclear Quadrupole Resonance (NQR) – Theory and its applications.

SEMESTER IV - THEORY PAPER

PAPER – III

CORE COURSE CODE - CHE 523

Course Credit = 04
(40 Lectures)

Selected Topics in Inorganic Chemistry

UNIT- I

(i) Electron Microscopy
SEM (Scanning electron microscopy), and TEM (Transmission electron microscopy).

UNIT- II

(ii) Electron Microscope AFM (Atomic force microscopy) STM (Surface tunneling microscopy).

UNIT- III

Photochemistry of Transition Metal complexes
Photoreactions of inorganic complexes.

UNIT- IV

Electrochemical Methods
Cyclic voltammetry.

UNIT- V

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

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 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.

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 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.

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 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.

SEMESTER III - THEORY PAPER

CORE COURSE CODE - CHE 513

Course Credit = 04
(40 Lectures)

PAPER - II

Oxidation, Reduction and Organometallic Reagents

UNIT-I

Oxidation
Hydrocarbons-alkenes, aromatic, rigns, saturated, C-H groups (activated and un-activated), 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.

SEMESTER III - THEORY PAPER

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

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 IV - THEORY PAPER
(Specialization in Organic Chemistry)

CORE COURSE CODE – CHE 524

PAPER – I

Biosynthesis and Chemistry of Natural Products

Course Credit = 04
(40 Lectures)

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.

SEMESTER IV - THEORY PAPER

PAPER –II

CORE COURSE CODE – CHE 525

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

SEMESTER IV - THEORY PAPER

PAPER –III

Course Credit = 04
(40 Lectures)

CORE COURSE CODE - CHE 526

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)

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

SEMESTER I - THEORY PAPER

CORE COURSE CODE: CHE 503 – PHYSICAL CHEMISTRY

Paper – III

Course Credit = 04
(40 Lectures)

UNIT – I

Partial Molar Properties, Nernst Heat Theorem (NHT) and Third Law of Thermodynamics

Nernst Heat Theorem and its application to non-condensed systems, Statements of the Third Law of Thermodynamics, Derivation of unattainability of absolute zero, The relationship between entropy constant and Nernst chemical constant, Determination of entropy from the Third Law using the correction due to gas imperfections.

UNIT – II

Statistical Mechanics

Quantum states and complexions, The combinatory rule, System with definite total energy, Degeneracy of energy levels, Probability and most probable distribution, Indistinguishability, 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

Spectroscopy

Molecular Spectra- Basic concepts of molecular spectroscopy, Classification of spectra, Characterization of electromagnetic radiations, Regions of the spectrum,

Rotation Spectra- Rigid and non-rigid rotation spectra-selection rule, Centrifugal distortion, Isotopic shift, Spectra of polyatomic molecules, Rotational constant, Experimental techniques.

UNIT – IV

Vibration rotation spectra- Simple harmonic oscillator, Vibrational energy,Anhormonicity, principle of vibration-rotation spectra, selection rule, PQR branches, Vibration in polyatomic molecules, Effect of nuclear spin, Isotopic shift, group frequency, Experimental techniques.

UNIT – V

Chemistry of Macromolecules

Introduction of type of polymers, Step polymerization, Kinetics of step polymerization, Statistical approach to Gelation, Molecular weight distribution in linear polycondensation (Derivation of size distribution), Molecular weight averages, Method of determining the molecular weight by osmotic pressure, Light scattering, Sedimentation and Viscosity methods.

SEMESTER – I PRACTICALS – LAB COURSE

PHYSICAL CHEMISTRY (in addition to Core Course Code CHE 503)

LAB COURSE CODE CHE 535

Course Credit = 02
(40 hrs)

1. Determine the concentration or percentage of one or two optically active substances in the given solution polarimetrically.

2. Kinetics of oxidation of reducing sugars by potassium ferricyanide/ copper(II) in presence of ammonium hydroxide or sodium hydroxide.

3. Kinetics of oxidation of alcohols/diols by aqueous alkaline hexacyanoferrate (III) ions.

4. Potentiometric titration of weak/strong acid and strong /weak base.

SEMESTER II - THEORY PAPER

COURSE CODE: CHE 507 – PHYSICAL CHEMISTRY

Paper – III

Course Credit = 04
(40 Lectures)

UNIT-I

Quantum Chemistry : Origin of quantum theory, Black body radiation, Wien and Rayleigh-Jeans laws, Planck's law and energy of harmonic oscillator

Postulates of quantum mechanics, Three dimensional time independent Schrodinger wave equation, Eigen functions and eigen values, Normalization and Orthogonality conditions, One dimensional harmonic oscillator, Tunnel effect, Eigen function and eigen value of H-atom (Solutions not required), shapes of s, p, d and f- orbitals
Approximate Methods- Variation principle and its application to ground state H-atom, Radial and Angular distribution curves for H-atom

UNIT-II

Chemical Kinetics : Thermodynamic formulation of rate constant, Comparison of collision and absolute reaction rate theories, Calculation of transmission coefficient, Transition State Theory in Solution, Primary and Secondary salt effects in the light of mechanistic tests, The theory of Absolute reaction rates - for reactions between atoms and reactions between molecules in terms of partition function, Influence of ionic strength and dielectric constant, Explosive reactions.

UNIT- III

Photochemistry - Premary and secondary processes in photochemistry, Fate and properties of excited states, Photolumineseence and Photostationary state, Photosensitization, Rice – Herzfeld mechanisms. Photochemical chain reactions (hyderogen and chlorine, hydrogen and bromine) Non-chain photochemical reactions (formation of phosgene, decomposition of H_2O_2 in presence of CO).

UNIT-IV

Electrolytes

Limitation of Arrhenius theory of electrolytic dissociation, Role of solvent and inter-ionic forces, activities and activity coefficients, determination of activity coefficients, Debye-Huckel Theory of the structure of dilute ionic solution, charge density and electrical potential, Properties of ionic cloud, activity coefficients from Debye-Huckel theory, Limiting law and its verification, Debye-Huckel Theory to more concentrated solutions, Partial molar quantities of electrolytic soltutions, determination of partial molar volume.

UNIT- V

Solid State

Crystal structures, Symmetry, Bonding in solids, Miller indices, Bragg's equation, X-ray analysis of NaCl.

SEMESTER – II PRACTICAL – LAB COURSE

PHYSICAL CHEMISTRY (in addition to Core Course Code CHE 507)

LAB COURSE CODE AGR. CHE 539

Course Credit = 02
(40 hrs)

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

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

3. Determination of density of refractive index of binary mixtures of acetone + CCl_4 at different compositions and calculation of partial molar volumes.

4. Conductometric/potentiometric titration of mixture of acids; KCl and KI etc.

SEMESTER III - THEORY PAPER

CORE COURSE CODE - CHE 515

Course Credit = 04
(40 Lectures)

PAPER – I

UNIT-I

Distribution law (Barometric formula), Sedimentation equilibrium, Maxwell's law of distribution of velocity and energy, Maxwell's law and Gaussian density function, 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.

UNIT-III

Indistinguishbility of gas molecules, 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, Heat capacities of crystals at very low temperatures.

UNIT-IV

Calorimetric entropy, Spectroscopic entropy , Comparison of calorimetric and Spectroscopic entropies, 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, Equilibrium constants of simple system-(i) Ionization of metal atoms, (ii) Dissociation of diatomic molecules and (iii) Isotopic exchange equilibria.

UNIT-V

Calculation of thermodynamic properties from spectroscopic data, Bose-Einstein stastics, Fermi Dirac Statistics, Comparison of M-B, B-E and F-D statistics, Fermi-Dirac gas (Electron gas in metals)- Bose —Einstein gas (liquid Helium).

SEMESTER III - THEORY PAPER

CORE COURSE CODE –CHE 516

Course Credit = 04
(40 Lectures)

PAPER – II

UNIT-I

Magnetic susceptibility and its determination, susceptibility equivalents, Pascal's law and its applications, 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

Orbital and spin moments, Electrons and multielectron systems, Magnetic property of complex compound in relation to their structure, Bohr magneton, L-S and J-J couplings. Electronoic spectra of molecules, Born-Oppenheimer approximation, Franck-Condon principle, Rotational fine structure of Electronic-Vibration transitions, Predissociation spectra, Molecular photoelectron spectroscopy (PES).

UNIT-III

Quantum theorty of Raman Spectra, Stokes and Antistokes lines, Rotation and vibration Raman spectra, Mutual exclusion principle, Laser Raman spectra, Theory of NMR relaxation process and chemical shift, The coupling constant, Nuclear spin interaction, Principle of ESR, Magnetic moment of electron and splitting factor, Hyper-fine splitting and double reasonance in ESR.

UNIT- IV

Mossbauer spectroscopy and its principle, Origin of line width, Isomer shift, Quadropole effects, Application of Raman, ESR, NMR and Massbaur spectra, C^{13} NMR spectroscopy, P^{31} NMR spectroscopy STM (Scanning Tunneling Microsocpy)-theory and application, AES (Auger Electron Spectroscopy), EELS (Electron Energy Lom Spectroscopy)

UNIT-V

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

SEMESTER III - THEORY PAPER

CORE COURSE CODE - CHE 517

Course Credit = 04
(40 Lectures)

PAPER – III

UNIT-I

Kinetics of fast reactions : Techniques of study of fast reactions with reference to stop flow, T-Jump, Flash photolysis 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, Phenamenological equations, Microscopic reversibility and Onsager's reciprocity relations.

UNIT-III

Transformations of the generalized fluxes and forces, Electrokinetic phenomena, Diffusion, Electric conduction, The stationary non-equilibrium states, States of minimum entropy production.

UNIT-IV

Nature of intermolecular forces, Linear oscillating dipoles, Various contributions of intermolecular forces, London theory of dispersion forces, Portetion function for system of independent particks, Thermodynamics of atomic crystals

UNIT-V

Partition function for system of dependent particles, partition functions (pressure, free energy and fugacity) of imperfect gas, Generalized model of imperfect gas and L-J potential and evaluation of second viral coefficient.

SEMESTER III - PRACTICALS CHEMISTRY

LAB COURSE CODE-PHYSICAL CHE- 543

(In addition to CHE CODE - 515, 516 & 517)

Course Credit = 04

(40 Lectures)

1. Oxidation of diols by cerium(IV) sulphate in acidic medium catalyzed by rhodium(III) chloride.

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

3. Uncatalyzed and/or iridium (III) catalyzed oxidation of arsenic (III) with alkaline hexacyanoferrate (III).

4. Determination of viscosity and density of aqueous solution of glucose/sucrose/urea at different temperatures and to calculate apparent and partial molar volume.

5. Determination of molecular weight of some electrolytes and non-electrolytes cryoscopically.

SEMESTER IV - THEORY PAPER

PAPER –I

CORE COURSE CODE - CHE 528

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, Thermodynamic functions of mixing of non-ideal solutions, 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, Wilson model and Flory-Huggins theory.

UNIT- III

Concept of operators in quantum mechanics—operators for velocity, kinetic energy, momentum and angular momentum, Detivation of Heisenberg's uncertainty principle, Solution for Hydrogen atom, Born-Oppenheimer approximation, Valence bond theory and its application to homonuclear (Hydrogen) and heteronuclear (HCl) diatomics, LCAO-MO treatment of hydrogen molecule ion, Comparative study of MO and VB theory.

UNIT- IV

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), Perturbation methods in LCAO-MO theory, Extended Huckel molecular orbital theory and SCF-MO method,

UNIT- V

Properties of colloids, sol-Gul transformation formation, colloidal electrolytes, Micellization and surfactants.

SEMESTER IV - THEORY PAPER

PAPER –II

Course Credit = 04
(40 Lectures)

CORE COURSE CODE - CHE 527

UNIT- I

Lattice energy of crystals, Cohesive energy, Conduction in solids and superconductance, Electronic structures of solids, Free electron theory, Fermi-gas theory and band theory of solids, Metals, semi-conductors and insulators, Intrinsic extrtinsic p-tyipe and n-type semi-conductors,

UNIT- II

Vapour pressure, compressbility viscosity and sound velocity, Internal pressure and its determination, Significance of internal pressure, solubility parameter and cohesive-energy-density, 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, Equation of state in terms of partition function, Outline of the theory of liquid state:JSimple cell theory (Eyring equation) and cell model theory of Lennard-Jones and Devonshire, Eyring's free volume theory of liquid viscosity, Effect of pressure on viscosity,

Thermodynamic functions of ideal and non-ideal liquid mixtures, Partial molar properties of liquid mixtures, Determination of partial molar volume and partial molar enthalpy,

UNIT- IV

The triumph and limitations of Debye-Huckel theory of activity coefficients, Electrical potential and mean activity coefficient in the case of ionic clouds with finite sized ions, The ion size parameter and comparison of the finite-ion-size model with experiment,

Asymmetry and electriphoretic effects, Stoke's law and Walden product, Debye-Huckel-Onsager equation, Conductance ratio and the Onsager slope, Verification of Debye-Huckel-Onsager equation, Conductivity of weak electrolytes and conductance in nonaqueous solvents, Modifications of Debye-Huckel-Onsager equation, Fuoss-Onsager and other equations, Wien and Debye-Fakenhagen effects.

UNIT- V

Viscosity of electrolyte solutions-Jones-Dole equation and significance of A and B coefficients, Ion association in an electrolyte solution, Formation of pairs, triplets etc,

The probability of finding oppositely charged ions near each other, Bjerrum theory of ion association,

SEMESTER IV - THEORY PAPER

PAPER –III

CORE COURSE CODE – CHE 529

Course Credit = 04
(40 Lectures)

UNIT- I

Heterogeneous catalysis, Kinetics and mechanism of reactions on surface, Mechanism of surface reactions, Uni and bi-molecular surface reactions, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Inhibition of surface reactions, Absolute reaction rate theory of surface reactions.

UNIT- II

Comparisoon of homogeneous and heterogenous reactions, Study of equilibrium constant and steady state treatment for Arrhenius and Vant Hoff's complexes, Influence of substituents on reaction rates (inductive and electromeric effects), Linear free energy relation ship, Taft equation, compensation effect, Hemmett acidity tunetions.

UNIT- III

a) Oxidation of sugars by $K_3Fe(CN)_6$ and Cu^{+2} in alkaline medium,
(b)Uncatalyzed and platinuem group metals (Osunium, ruthenium, iridium, palladium, rhodium etc.) Catalyzed oxidation of organic and inorganic compounds by $K_3Fe(CN)_6$ and Ce (IV) etc in acidic / alkaline medium.

UNIT- IV

Kinetic of initiation retardation, chain polymerization and ionic polymerization (anionic and cationic), Copolymerisation (with special reference to monomer reactivites ratios).

UNIT- V

Coordination polymerization, Degradation of polymers (oxidative, chemical and photolytic), An introduction to conducting polymers, Polyelectrolytesn.

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 the oxidation of cyclic alcohols by cerium(IV) sulphate in acidic medium in presence of Iriduum(III) chloride.

2. Kinetics of iridium (III) catalyzed oxidation of aromatic aldehydes/aromatic alcohols/hydrocarbons by cerium (IV) in aqueous acidic medium.

3. Kinetics of Ru(III) catalysed oxidation of alcohols/diols by Ce(IV) sulphate in acidic medium .

4. Kinetics of oxidation of aliphatic/cyclic alcohols/glycols by alkaline hexacyanoferrate(III) catalyzed by ruthenium (III) chloride.

SEMESTER III - ELECTIVE PAPER

ELECTIVE COURSE CODE – CHE 551

Course Credit = 04
(40 Lectures)

PAPER – IV

Solid – State and Nuclear Chemistry

(40 Lectures)

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.

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. DEPT,INEPT,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 spectrometery Examples of mass spectral fragementation 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.

SEMESTER III - ELECTIVE PAPER

ELECTIVE COURSE CODE – CHE 553

PAPER – IV

Course Credit = 04
(40 Lectures)

Biophysical Chemistry

Thermodynamics Of Biochemical System

Different types of chemical process accounting in living systems, Relation between microscopic and macroscopic dissociation constants (acid dissociations of amino acids), Calculation of binding curves binding of protons by phosphate), Relationship between number of ligands bond per molecule of base and the partition function, Bioenergetic thermodynamics , Role of ATP in biological systems , Themodynamics of hydrolysis of adenosine triphosphate (ATP), Standard Gibbs free energies of a number of phosphate esters, Binding of oxygen by Myoglobin and hemoglobin,

Photochemistry and photobiology

Introduction, Photosynthesis , Chlorophyll molecules , Photosystems I and II, Biochemical reactions ,Vision , Rotation about C-C and C=C bonds , Mechanism of vision , Chemiluminescence and Bioluminescence , UV irradiation of DNA

Statistical mechanics in biopolymers

Chain configuration and conformations of macromolecules , Proteins , Polypeptide structure , Protein folding problems

SEMESTER III - ELECTIVE PAPER

ELECTIVE COURSE CODE – CHE 554

Course Credit = 04
(40 Lectures)

PAPER IV

Environmental Analysis / Monitoring

UNIT-I

Water quality standards; Sampling and measurements of parameters like DO, BOD, COD, TOC, pH, Total Suspended Solids, Total Dissolved Solids, Hardness, Amount of Organic Matters, pE Determination of Inorganic ions, Plant Nutrients, NKP

UNIT-II

Methods of removal of Heavy Metals and Dyes from the polluted water

UNIT-III

Analysis of Waste Water- Monitoring of Soaps, Detergents and Pesticides in waste water, Sampling and Measurement of Air Pollutants, Monitoring automobile Emissions, Monitoring Emissions from Stationary Sources.

UNIT-IV

Monitoring Particulate Emissions (High – Volume sampling, Separation of Particles by size, XRF Spectrometry)

UNIT-V

Monitoring of Disease – Causing Agents, Microbiological tests for coliform, Multiple – Tube Fermentation Technique, Membrane Filtration Technique Ortho – nitrophenyl – β – D – galactopyranoside (ONPG) Test.

SEMESTER IV - ELECTIVE PAPER

PAPER – I

ELECTIVE COURSE CODE – CHE 555

Course Credit = 04
(40 Lectures)

Environmental 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)

SEMESTER IV - ELECTIVE PAPE

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

SEMESTER IV - ELECTIVE PAPER

PAPER – III

ELECTIVE COURSE CODE – CHE 557

Course Credit = 04
(40 Lectures)

Nano-Catalysis

UNIT : I

Introduction, classification of nanomaterials, preparation and characterization, different types of nanostructures- nanoparticles, nanoclusters, nanowires, nanorods, nanofilms, nanotubes, C-nanotubes etc

UNIT : II

Chemical activity, selectivity and specificity of nanocatalyst, role of size, shape and surface area of nanoparticles in catalysis. Bulk and nanoscale surfaces, chemical reactions on point defects on oxide surfaces.

UNIT : III

Chemical reactions and catalytic processes on free and supported clusters, catalytic processes on free metal clusters, chemical reactions and catalytic cycles on supported clusters. single atoms on oxide surfaces, size -selected clusters on oxide surfaces, size -distributed clusters en oxide surfaces.

UNIT : IV

Mode of action of catalysts, classification & comparison-homogeneous and heterogeneous catalysis, Mechanism: intermediate steps and kinetics of homogeneous and heterogeneous processes, Langmuir Hinshelwood mechanism for nanocatalyst.

UNIT : V

Techniques to determine the properties of nanocatalysts like TEM, XRD. Applications of nanocatalysis in pharmaceutical, in synthesis of fine chemicals, in medicine for protection of environment etc.

SEMESTER IV - ELECTIVE PAPER

PAPER – IV

ELECTIVE COURSE CODE – CHE 558

Course Credit = 04
(40 Lectures)

Nuclear Chemistry and Radiochemical Analysis

UNIT - I

Fundamentals of Nuclear Chemistry, Stability of nucleus, Properties of nucleus, Nuclear Models.

UNIT - II

Nuclear reactions – fission, fusion, spallation, fragmentation, stripping and pick up reactions, photonuclear and thermonuclear reactions.

UNIT - III

Interaction of Radiation with matters : Counting techniques and counting statistics, Ionisation, Propertional GM and scintillation counters, counting errors and corrections, Chemical Dosimetry.

UNIT - IV

Activation Analysis Tracer Techniques and Dilution Analysis, Radiometric titrations.

UNIT - V

Radiocarbon and other dating