APPLICATION OF SPECTROSCOPY-II (Compulsory)

CHE401

UNIT-I

Ultraviolet and Visible spectroscopy

Various electronic transitions (185-800 nm) Beer-Lambert law, Effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in biphenyls.

UNIT-II

Infrared Spectroscopy

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance.

UNIT-III

Nuclear Magnetic Resonance of Paramagnetic Substances in Solution

The contact and Pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclide with emphasis on ^{195}Pt and ^{119}Sn NMR.

UNIT-IV

Carbon-13 NMR Spectroscopy

General considerations, chemical shift (aliphatic olefinic, alkyne, aromatic, heteroaromatic and carboynl carbon), coupling constants. Two dimension NMR spectroscopy-COSY, NOESY, DEPT, HMBC and HMQC techniques.

UNIT-V

Mass Spectrometry

Introduction ion production E1, C1 FD, ESI and FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Me Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Structure elucidation of simple molecules using UV – Visible, IR, NMR and mass spectral techniques.

Suggested Readings:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectral : Inorganic and Coordination Compounds K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15 ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry ed. R.L. Carlin vol. 3 dekker.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.

SOLID STATE CHEMISTRY (Compulsory)

CHE402

UNIT-I

Solid State Reactions

General principles, experimental procedure, co-precipitation as a precursory to solid state reactions, kinetics of solid state reactions.

UNIT-II

Crystal Defects and Non-Stoichiometry

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky detects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colourcentres, non-stoichiometry and defects.

UNIT-III

Electronic Properties and Band Theory

Metals insulators and semiconductors, electronic structure of solidsband theory band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors. Optical properties-Application of optical and electron microscopy. Magnetic Properties-Classification of materials : Effect of temperature calculation of magnetic moment, mechanism of ferro and anti ferromagnetic ordering super exchange.

UNIT-IV

Organic Solids
Electrically conducting solids. organic charge transfer complex, organic metals, new superconductors.

UNIT-V

Liquid Crystals:

Types of liquid crystals: Nematic, Smectic, Ferroelectric, Antiferroelectric, Various theories of LC, Liquid crystal display, New materials.

Suggested Readings:

1. Solid state chemistry and its applications, A.R. West. Peenum.
2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

BIOCHEMISTRY (Compulsory)

CHE403

UNIT-I

Metal Ions in Biological Systems
Bulk and trace metals with special reference to Na, K, Mg, Ca, Fe, Cu, Zn, Co, and K+/Na+ pump.
Bioenergetics and ATP Cycle.
DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophyll's, photosystem I and photosystem II in cleavage of water.

Transport and Storage of Dioxygen Heam proteins and oxygen uptake structure and function of haemoglobin's, mygolobin, haemocyanms and hemerythrin, model synthetic complexes of iron, cobalt and copper.

UNIT-II

Electron Transfer in Biology

Structure and function of metal of proteins in electron transport processes cytochrome's and ion-sulphure proteins, synthetic models. **Nitrogen fixation** Biological nitrogen fixation, and its mechanism, nitrogenase, Chemical nitrogen fixation.

UNIT-III

Enzymes
Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshalnd'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 kinetics, Michael's-Menten and Lineweaver Burk plots, reversible and irreversible inhibition. **Mechanism of Enzyme Action** Transition-state theory, orientation and Steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chemotrypsin, ribonuclease, lysozyme and carboxypeptidase.

Kinds of Reactions Catalysed by Enzymes Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in Isomerisations reactions, b-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

UNIT-IV

Co-Enzyme Chemistry

Cofactors as derived from vitamines, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors. **Enzyme Models**

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and

prochirality Biometric chemistry, crown ether, cryptates. Cyclodextrins, cyclodextrion-based enzyme models, clixarenes, ionospheres, micelles synthetic enzymes or synzymes.

Biotechnological Applications of Enzymes

large-scale prodcution and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from cron starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

UNIT-V

Biological Cell and its Constituents

Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coils transition.

Bioenergetics

Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Biopolymer Interactions

Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibrium and various types of bidning processes in biological systems. Hydrogen ion titration curves.

Cell Membrane and Transport of Ions

Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

Suggested Readings:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic biochemistry vol. I and II ed. G.L. Eichhorn, Elsever.
4. Progress in Inorganic Chemistry, Vol 18 and 38 ed J.J. Lippard, Wiley.
5. Bioorganic Chemistry : A chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.

6. Understanding Enzymes, Trevor Palmer, Prentice Hall.

7. Enzyme Chemistry : Impact and applications, Ed. Collin J suckling, chemistry.

8. Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry.

9. Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press.

MEDICINAL CHEMISTRY (OPTIONAL)

CHE404 (A)

UNIT-I

Structure and activity : Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

UNIT-II

Pharmacodynamics:

Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

UNIT-III

Antibiotics and antibacterials

Introduction, Antibiotic β-Lactam type - Penicillins, Cephalosporins, Antitubercular – Streptomycin, Broad spectrum antibiotics – Tetracyclines, Anticancer - Dactinomycin (Actinomycin D)

UNIT-IV

Antifungal –

polyenes, Antibacterial – Ciprofloxacin, Norfloxacin, Antiviral – Acyclovir

Antimalarials:Chemotherapy of malaria. SAR. Chloroquine, Chloroguanide and Mefloquine

UNIT-V

Non-steroidal Anti-inflammatory Drugs :

Diclofenac Sodium, Ibuprofen and Netopam

Antihistaminic and antiasthmatic agents :

Terfenadine, Cinnarizine, Salbutamol and Beclomethasonedipropionate.

Suggested Readings:

1. Introduction to medicinal chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age Internaitonal.
4. Burger's Medicianl Chemistry and Drug Discovery, Vol-I (Chapter 9 and Chapter 14), Ed. M.E.Wolff, John Wiley.
5. Goodman and Gilman's Pharmacoloical Basis of Therapeutics, Mc GRaw-Hill.

ELECTROCHEMISTRY

CHE-404 (B)

UNIT-I

1. Conversion and Storage of Electrochemical Energy Present status of energy consumption :
Pollution problem. History of fuel cells, Direct energy conversion by electrochemical means. Maximum intrinsic efficiency of an electrochemical converter. Physical interpretation of the Carnot efficiency factor in electrochemical energy converters. Power outputs.
electrochemical Generators (Fuel Cells) : Hydrogen oxygen cells, Hydrogen Air cell, Hydrocarbon air cell, Alkane fuel cell, Phosphoric and fuel cell, direct NaOH fuel cells, applications of fuel cells.

2. Electrochemical Energy Storage :

Properties of Electrochemical energy storage : Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries : (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries : (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium Battery, Future Electricity storers : Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

UNIT-II

Corrosion and Stability of Metals :

Civilization and Surface mechanism of the corrosion of the metals; Thermodynamics and the stability of metals, Potential -pH (or Pourbaix) Diaphragmsl; uses and abuses, Corrosion current and corrosion potential -Evans diagrams. Measurement of corrosion rate : (i0 Weight Loss method, (ii) Electrochemical Method.

Inhibiting Corrosion :

Cathodic and Anodic Protection. (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by charging the corroding method from external source, anodic Protection, Organic inhibitors, The fuller Story Green inhibitors.

Passivation :

Structure of Passivation films, Mechanism of Passivation, Spontaneous Passivation Nature's method for stabilizing surfaces.

UNIT-III

Bioelectrochemistry :
bioelectrodics, Membrane Potentials, Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Kinetic of Electrode Process :

Essentials of Electrode reaction. Current Density, Overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K0) and Transfer coefficient (a), Exchange Current.

Irreversible Electrode processes : Criteria of irreversibility, informatino from irreversible wave.

UNIT-IV

Methods of determining kinetic parameters for quasi-rversible and irreversible waves : Koutecky's methods, Meits Israel Method, Gellings method

Electrocatalysis :
Chemical catalysts and Electrochemical catalysts with special reference to purostates, porphyrin oxides of rare earths. Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. Influence of various parameters.

UNIT-V

Potential Sweep Method :

Linear sweep Voltammetry, Cyclic Voltammetry, theory and applications. Diagnostic criteria of cycli voltammetry. Controlled current microelectrode techniques : comparison with controlled potentials methods, chronopotentiometry, theory ad applications.

Bulk Electrolysis Methods :

Controlled potential coulometry, Controlled Coulometry, Electroorganic synthesis and its important applications. Stripping analysis : anodic and Cathodic modes, Pre electrolysis and Stripping steps, applications of Stripping Analysis.

SUGGESTIED READINGS:

1. Polarographic Techniques by L. Meites, Interscience.
2. "Fuel Cells : Thjeir electrochemistry". McGraw Hill Book Company, New York.
3. Modern Polarographic Methods by A.M. Bond, Marcell Dekker.
4. Polarography and allied techniques by K. Zutshi, New age International publicatin. New Delhi.

INDUTSTRIAL CHEMISTRY - PESTICIDES & GLASS INDUSTRIES (OPTIONAL)

CHE405 (A)

UNIT-I

Cleansing Agents

Cleansing Agents : Toilet and washing soaps; preparation and uses, Synthetic detergents; alkyl aryl sulfonates, fatty alcohot surfaces, ethanolamines, nonionic detergents.

UNIT-II

Fertizilizers and Inorganic Materials :

Fertilizers : Fertilizers Industries in India, Manufacture of Ammonium salts. Urea, Nitrates, Phosphates and Supephosphates, Nitrogen fixation.

Glass: Types, their composition and properties testing glass. Manufacture of Glass Fibres.Optical Glass, Coloured Glasses, Lead Glass and Neutron Absorbing Glass.

Ceramics: Important clays and feldspar. Glazing and vitrification, Glass ceramics.

UNIT-III

Cement : Types and their manufacture, setting process.

Ferrous Industry: Manufacture of steel and other important alloys.

Silicon : Pre silicon, Electronics Industry.

UNIT-IV

Pesticies and Food additives

Pesticies and Food additives : Classification, important categories of insecticides, fungicides, herbicides and rodenticies; Mode of action.

UNIT-V

Chemistry and synthesis of common pesticides : Such and Tabun, Sarin, Daygon, DDYP paraquat.

Suggested Readings:

Industrial Chemistry J.S Jangwan, A. S Mathuria

CHEMISTRY OF NATURAL PRODUCTS

CHE-405 (B)

UNIT-I

Terpenoids and Carotenoids

Calsifications, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules : Citral, Geraniol -Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and -Carotene.

UNIT-II

Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : Ephedrine , (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.

UNIT-III

Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone, Biosynthesis of Steroids.

UNIT-IV

Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin Quercetin, Myrcetin, Quercetin 3-glucoside, Vitexin, Diadzein, Aureusin, Cyanidin-7arabinoside, Cyanidin, Hirsutidin, Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Prophyrins

Structure and synthesis of Haemoglobin and Chlorophyll.

UNIT-V

Prostaglandin

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2a.

Pyrethroids and Rotenones

Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

SUGGESTED READINGS:

1. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers.
2. New Trends in Natural Product chemistry, Ataaur Rahman and M.L. Choudhary, Harwood Academic Publishers.
3. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
4. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. harwood Academic Publishers.
5. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

Chemistry

Practical

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry	**Max Marks - 33**
Preparation	**12**
Spectrophotometric Determinations	
Flame Photometric Determinations	12
Record	04
Viva Voice	**05**
Total	**33**

Preparation

Preparation of selected inorganic compounds and their study by IR, electronic spectra, and magnetic

susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following :

1. Sodium amide. Inorg. Synth., 1946, 2, 128.
2. Atomic absorption analysis of Mg and Ca.
3. Synthesis of trichlorodiphenylantimony (V) hydrate. Inorg. Synths., 1985, 23, 194
4. Sodium tetrathionate $Na_2S_4O_6$.
5. Metal complex of dimethyl sulfoxide : $CuCl_2$.2DMSO J.Chem. Educ., 1982, 59, 57.
6. Synthesis of metal acethylacetonate :Inorg. Synths, 1957, 5, 130, 1963, 1, 183.
7. Cis and Trns $[Co(en)_2CI_2]^+$.
8. Determination of Cr (III) complex. $[Cr(H_2O)_6]NO_3$.3HO,.Inorg. synths., 1972, 13, 184.
9. Preparation and use of Ferrocene. J. Chem. Edu. 1966, 43, 73; 1976, 53, 730.
10. Preparation of [Co(phenathroline-5,6 quinone)].

Spectrophotometric Determinations / Spectroscopic identification of recorded spectra like IR, NMR, ESR and Mass

a. Manganese/Chromium in steel sample.
b. Nickel by extractive spectrophotometric method.
c. Fluoride/nitrite/phosphate.
d. Copper-Ethylene diaminecomplex : Slope-ratio method.

Flame Photometric Determinations

a. Sodium and potassium when present together.
b. Lithium/calcium/barium/strontium.
c. Cadmium and magnesium in tap water.

Organic Chemistry	**Max Marks - 33**
Multi-step Synthesis of Organic Compounds	**12**
Spectroscopy/Spectrophotometric Determinations	12
Record	**04**
Viva Voice	**05**
Total	**33**

Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. Photochemical reaction Benzophenone ->Benzpinacol _>Benzpinacolone Beckmann rearrangement :Benzanilide from benzene Benzene ->Benzophenone ->Benzphenoneoxime ->BenzanilideBenzilic acid rearrangement : Benzilic acid from benzoin Benzoin ->Benzil ->Benzilic acid Synthesis of heterocyclic compounds Skraup synthesis : Preparation of quinoline from aniline Fisher Indole synthesis : Preparation of 2-phenylindole from phenylhydrazine. Enzymatic synthesis Enzymatic

synthesis Enzymatic reduction : reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ehtyl-3-hydroxybutanoate and determine its optical purity. Biosynthesis of ethanol from sucrose.Synthesis using microwave Alkylation of diethyl malonate with benzyl chloride.Synthesis using phase transfer catalyst.Alkylation of diethyl malonate or ethyl acetoacetate with an alkylhalide.

Spectroscopy
Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

Spectrophotometric (UV/VIS) Estimations/isolation of the following (any one compound)

Spectroscopic estimation

1. Amino acids
2. Proteins
3. Carbohydrates
4. Ascorbic acid
5. Aspirin
6. Caffeine

Isolation

1. Casein from milk
2. Lycopine from tomato
3. Piperine from black pepper
4. Caffeine from tea leaves
5. Lactose from milk

Physical Chemistry	**Max Marks - 34**
Experiment No. 1	**13**
Experiment No. 2	**12**
Record	**04**
Viva Voice	**05**
Total	**34**

Spectroscopy

i. Determination of PKa of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.

ii. Determination of stoichiometry and stability constant of Ferricisothicoyanation complex ion in solution.

iii. Determination of rate constant of alkaline bleaching of Malachite green and effect of ionic strength on the rate of reaction.

Chemical Kinetics

i. Determination of rate constant and formation constant of an intermediate complex in the reaction of Ce(IV) and Hypophosphorous acid at ambient temperature.

ii. Determination of energy and enthalpy of activation in the reaction of KMnO4 and benzyl alcohol in acid medium.

iii. Determination of energy of activation of and entropy of activation from a single kinetic run.

iv. Kinetics of an enzyme catalyzed reaction.

Thermodynamics

i. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.

ii. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intromolecular in tetractions (benzoic acid in water and in DMSO water mixture and calculate the partial molar heat of solution.

iii. **Polarography**

i. Identification and estimation of metal ions such as Cd+2, Pb+2, Zn+2, and i+2 etc. polarographically.

ii. Study of a metal ligand complex polarographically (using Lingane's Method).