

UNIVERSITY OF MUMBAI

No. UG/85 of 2018-19

CIRCULAR:-

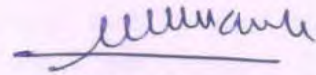
Attention of the Principals of the affiliated Colleges, the Head University Departments and Directors of the recognized Institutions in Science & Technology Faculty is invited to this office Circular Nos. UG/226 of 2006, dated 29th June, 2006 relating to syllabus of the Master of Science (M.Sc.) degree course.

They are hereby informed that the recommendations made by the Board of Studies in Chemistry at its meeting held on 28th May, 2018 have been accepted by the Academic Council at its meeting held on 14th June, 2018 **vide** item No. 4.71 and that in accordance therewith, the revised syllabus as per the (CBCS) for the M.Sc. in Organic Chemistry (Sem – III & IV), has been brought into force with effect from the academic year 2018-19, accordingly. (The same is available on the University's website www.mu.ac.in).

MUMBAI – 400 032

19th June, 2018

To



(Dr. Dinesh Kamble)

I/c REGISTRAR

The Principals of the affiliated Colleges, the Head University Departments & Directors of the recognized Institutions in Science & Technology Faculty. (Circular No. UG/334 of 2017-18 dated 9th January, 2018.)

A.C./4.71/14/06/2018

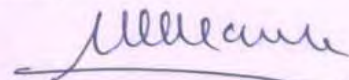
No. UG/ 85 -A of 2018

MUMBAI-400 032

19th June, 2018

Copy forwarded with Compliments for information to:-

- 1) The I/c Dean, Faculty of Science & Technology,
- 2) The Chairman, Board of Studies in Chemistry,
- 3) The Director, Board of Examinations and Evaluation,
- 4) The Director, Board of Students Development,
- 5) The Co-Ordinator, University Computerization Centre,



(Dr. Dinesh Kamble)

I/c REGISTRAR

AC - 14/06/2018

Item No. 4.71

UNIVERSITY OF MUMBAI



Program : M.Sc.

(Choice Based Credit System)

Course : M.Sc. Organic Chemistry

Part - I

Syllabus for Semester III & IV

(To be implemented from the Academic year 2018-2019)

M.Sc. Organic Chemistry

Semester – III

Course Code: PSCHO301

Paper - I (Theoretical organic chemistry-I)

Unit 1	Organic reaction mechanisms	[15L]
1.1	Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes.	[5L]
1.2	Neighbouring group participation: Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π -electrons, aromatic rings, σ -bonds with special reference to norbornyl and bicyclo[2.2.2]octyl cation systems (formation of non-classical carbocation)	[3L]
1.3	Role of FMOs in organic reactivity: Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the α effect.	[2L]
1.4	Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bond making and breaking Symmetry-Allowed and Symmetry-Forbidden Reactions – <ul style="list-style-type: none">• The Woodward-Hoffmann Rules-Class by Class• The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules <ul style="list-style-type: none">• The Aromatic Transition structures [Huckel and Mobius]• Frontier Orbitals• Correlation Diagrams, FMO and PMO approach Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5 hexatriene and allyl system.	[5L]
Unit 2	Pericyclic reactions	[15L]
2.1	Cycloaddition reactions: Supra and antra facial additions, $4n$ and $4n+2$ systems, $2+2$ additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. Other Cycloaddition Reactions- [4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.	[7L]
2.2	Electrocyclic reactions: Conrotatory and disrotatory motions, $4n\pi$ and $(4n+2)\pi$ electron and allyl systems.	[3L]
2.3	Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy-Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.	[5L]

Unit 3:	Stereochemistry-I	[15L]
3.1	Classification of point groups based on symmetry elements with examples (nonmathematical treatment).	[2L]
3.2	Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions.	[3L]
3.3	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes , steroids, and Bredt's rule.	[5L]
3.4	Anancomeric systems , Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones (with LiAlH₄, selectride and MPV reduction) and oxidation of cyclohexanols.	[5L]
Unit 4	Photochemistry	[15L]
4.1	Principles of photochemistry: quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.	[3L]
4.2	Photochemistry of carbonyl compounds: $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α , β -unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.	[8L]
4.3	Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π -methane rearrangement including aza-di- π -methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	[2L]
4.4	Photochemistry of arenes: 1, 2-, 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	[1L]
4.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	[1L]

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- 4 Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
- 5 Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
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 - 13 Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
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 - 25 Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
 - 26 Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
 - 27 Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
 - 28 Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
 - 29 Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
 - 30 Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
 - 31 Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
 - 32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.

- 33 Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
 34 Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
 35 Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
 36 Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
 37 Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication)

Course Code: PSCHO302

Paper-II

Synthetic Organic Chemistry-I

Unit 1:	Name reactions with mechanism and application	[15L]
1.1	Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Ester synthesis, Ritter reaction, Yamaguchi esterification, Peterson olefination.	[5L]
1.2	Domino reactions: Characteristics; Nazarov cyclization	[3L]
1.3	Multicomponent reactions: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, <u>Pictet-Spengler synthesis</u>	[5L]
1.4	Click Reactions: Characteristics; Huisgen 1,3-Dipolar Cycloaddition	[2L]
Unit 2:	Radicals in organic synthesis	[15L]
2.1	Introduction: Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	[3L]
2.2	Radical Initiators: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	[1L]
2.3	Characteristic reactions - Free radical substitution, addition to multiple bonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity), radical cyclizations, autoxidations: synthesis of cumene hydroperoxide from cumene.	[4L]
2.4	Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: $S_{RN}Ar$ reactions.	[4L]
2.5	Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	[3L]
Unit 3:	Enamines, Ylides and α-C-H functionalization	[15]
3.1	Enamines: Generation & application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.	[4L]
3.2	Phosphorus, Sulfur and Nitrogen Ylides: Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	[6L]

- 3.3 **α -C-H functionalization:** By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth–Gilbert homologation, Steven’s rearrangement. [5L]
- Unit 4: Metals / Non-metals in organic synthesis** [15]
- 4.1 **Mercury in organic synthesis:** Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents. [3L]
- 4.2 **Organoboron compounds:** Mechanism and regiochemistry of hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and functional group reduction by diborane. [3L]
- 4.3 **Organosilicons:** Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β -silyl cations as intermediates. Iodotrimethylsilane in organic synthesis. [3L]
- 4.4 **Silyl enol ethers:** Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions. [2L]
- 4.5 **Organotin compounds:** Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom. [2L]
- 4.6 **Selenium in organic synthesis:** Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as α -C-H activating groups [2L]

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- **Name Reactions**, Jie Jack Lie, 3rd Edn., Springer
- **Organic Electrochemistry**, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: PSCHO303

Paper-III

Natural products and Spectroscopy

Unit 1:	Natural products-I	[15L]
1.1	Carbohydrates: Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected). Structural features and applications of inositol, starch, cellulose, chitin and heparin.	[5L]
1.2	Natural pigments: General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β -carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxyacetophenone.	[5L]
1.3	Insect pheromones: General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex pheromones etc.), advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3-butadiene.	[3L]
1.4	Alkaloids: Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	[2L]
Unit 2:	Natural products-II	[15L]
2.1	Multi-step synthesis of natural products: Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations: a) Woodward synthesis of Reserpine from benzoquinone b) Corey synthesis of Longifoline from resorcinol c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene e) Synthesis of Juvabione from Limonene	[8L]

- f) Synthesis of Taxol.
- 2.2 **Prostaglandins:** Classification, general structure and biological importance. Structure elucidation of **PGE₁**. [2L]
- 2.3 **Lipids:** Classification, role of lipids, Fatty acids and glycerol derived from oils and fats. [2L]
- 2.4 **Insect growth regulators:** General idea, structures of JH₂ and JH₃. [1L]
- 2.5 **Plant growth regulators:** Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1-tetrahydropyranyloxydodecane expected). [2L]
- Unit 3: Advanced spectroscopic techniques-I [15L]**
- 3.1 **Proton NMR spectroscopy:** Recapitulation, chemical and magnetic equivalence of protons, First order, second order, Spin system notations (A₂, AB, AX, AB₂, AX₂, AMX and A₂B₂-A₂X₂ spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents. [7L]
- 3.2 **¹³C –NMR spectroscopy:** Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), ¹³C- chemical shifts, calculation of ¹³C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to ¹⁹F and ³¹P. [4L]
- 3.3 Spectral problems based on UV, IR, ¹HNMR and ¹³CNMR and Mass spectroscopy. [4L]
- Unit 4: Advanced spectroscopic techniques-II [15L]**
- 4.1 **Advanced NMR techniques:** DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE and NOESY techniques. [10L]
- 4.2 Spectral problems based on UV, IR, ¹HNMR, ¹³CNMR (Including 2D technique) and Mass spectroscopy [5L]

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Course Code: PSCHOEC-I 304

Paper-IV

Medicinal , Biogenesis and green chemistry

Unit 1:	Drug discovery, design and development	[15L]
1.1	Introduction, important terms used in medicinal chemistry: receptor, therapeutic index, bioavailability, drug assay and drug potency. General idea of factors affecting bioactivity: Resonance, inductive effect, bioisosterism, spatial considerations. Basic pharmacokinetics: drug absorption, distribution, metabolism (biotransformation) and elimination. Physical and chemical parameters like solubility, lipophilicity, ionization, pH, redox potential, H-bonding, partition coefficient and isomerism in drug distribution and drug-receptor binding.	[7]
1.2	Procedures in drug design: Drug discovery without a lead: Penicillin, Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: Identification of the pharmacophore, Functional group modification. Structure-activity relationship, Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain transformation, bioisosterism, combinatorial synthesis (basic idea).	[8L]
Unit 2:	Drug design, development and synthesis	[15L]
2.1	Introduction to quantitative structure activity relationship studies. QSAR parameters: - steric effects: The Taft and other equations; Methods used to correlate regression parameters with biological activity: Hansch analysis- A linear multiple regression analysis.	[5L]
2.2	Introduction to modern methods of drug design and synthesis- computer-aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.	[3L]
2.3	Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types of prodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Soft drugs: concept and properties.	[3L]
2.4	Synthesis and application of the following drugs: Fluoxetine, cetirizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	[4L]
Unit 3:	Biogenesis and biosynthesis of natural products	[15L]
3.1	Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.	[3L]

- 3.2 Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides. [4L]
- 3.3 Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids. [4L]
- 3.4 Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes. [4L]
- Unit 4: Green chemistry [15L]**
- 4.1 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. [1L]
- 4.2 Use of the following in green synthesis with suitable examples: [9L]
- a) Green reagents: dimethylcarbonate, polymer supported reagents.
- b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquat 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.
- c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide.
- d) Solid state reactions: solid phase synthesis, solid supported synthesis
- e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.
- f) Ultrasound assisted reactions.
- 4.3 Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole. [3L]
- 4.4 Green Catalysts : Nanocatalyst, Types of nanocatalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts. [2L]

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43. Organic synthesis in water. By Paul A. Grieco, Blackie.
44. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
45. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.
46. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Course Code: PSCHOEC-II 304

Paper-IV

Bioorganic chemistry

Unit 1:	Biomolecules-I	[15L]
1.1	Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α - helix, β -sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure.	[2L]
1.2	Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.	[3L]
1.3	Structure: Purine & pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation.	[3L]
1.4	RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA – general account , t- RNA-clover leaf model, Ribozymes.	[2L]
1.5	DNA: Physical properties – Effect of heat on physical properties of DNA (Viscosity, buoyant density and UV absorption), Hypochromism, Hyperchromism and Denaturation of DNA. Reactions of nucleic acids (with DPA and Orcinol).	[2L]
1.6	Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester,	[3L]

Phosphoramidite and H- phosphonate methods including solid phase approach.

Unit 2:	Biomolecules-II	[15L]
2.1	Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: a) enzyme efficiency/ catalytic power b) enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site.	[6L]
2.2	Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.	[4L]
2.3	Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond.	[5L]
Unit 3:	Biomolecules - III	[15L]
3.1	Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide, flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate, Vitamin B12, biotin, lipoic acid, Coenzyme A.	[12L]
3.2	Oxidative phosphorylation, chemiosmosis, rotary model for ATP synthesis and role of cytochrome in oxygen activation.	[3L]
Unit 4:	Biomolecules – IV	[15L]
4.1	Role of main enzymes involved in the synthesis and breakdown of glycogen.	[2L]
4.2	Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction.	[6L]
4.3	Enzymes in organic synthesis. Fermentation: Production of drugs/drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, β -lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde) and immobilized form (production of 6-aminopenicillanic acid).	[7L]

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47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Semester III: Practicals

Course code: PSCHO3P1

Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique

1. Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) (for solid mixture: water insoluble/ soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Identification of the two components (indicated by the examiner) using micro-scale technique.
3. Preparation of derivatives (any one of separated compound).

(Minimum 8 experiments)

Course code: PSCHO3P2

Single step organic preparation(1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography.

1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography)
2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation)
3. .Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography)

4. Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography)
5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation).
6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation).
7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation).
8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation)
9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography)
11. Preparation of fluorenone from fluorene. (Purification by column chromatography)
12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)

(Minimum 8 experiments)

Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

References for Practicals

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition, 2008,

B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.

11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.

12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.

2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Semester – IV

Course Code: PSCHO401

Paper - I (Theoretical organic chemistry-II)

Unit 1:	Physical organic chemistry	[15L]
1.1	Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ -values, reaction constants ρ , Yukawa-Tsuno equation.	[7L]
1.2	Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, σ_I and σ_R scales, steric parameters E_s and β . Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's E_T parameter, Solvatochromism Z-scale, Spectroscopic Correlations, Thermodynamic Implications.	[8L]
Unit 2	Supramolecular chemistry	[15L]
2.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	[3L]
2.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	[3L]
2.3	Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.	[5L]
2.4	Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gels and Fibres.	[4L]
Unit 3	Stereochemistry- II	[15L]

- 3.1 Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds. [3L]
- 3.2 Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). [3L]
- 3.3 Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy. [4L]
- 3.4 Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α -haloketone rule with applications. [5L]
- Unit 4: Asymmetric synthesis** [15L]
- 4.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions. [3L]
- 4.2 Synthesis of L-DOPA [Knowles's Monsanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins. [9L]
- 4.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations. [3L]

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- 2 A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
- 3 Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
- 4 Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
- 5 Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
- 6 Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
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- 21 Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006
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- 29 Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
- 30 Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
- 31 Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
- 32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
- 33 Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
- 34 Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
- 35 Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
- 36 Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.

Course Code: PSCHO402
Paper - II (Synthetic organic chemistry-II)

Unit 1:	Designing Organic Synthesis-I	[15L]
1.1	Protecting groups in Organic Synthesis: Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	[3L]
1.2	Concept of umpolung (Reversal of polarity): Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	[3L]
1.3	Introduction to Retrosynthetic analysis and synthetic planning: Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity.	[9L]
Unit 2:	Designing Organic Synthesis-II	[15L]
2.1	General strategy: choosing a disconnection-simplification, symmetry, high yielding steps, and recognisable starting material.	[3L]
2.2	One group C-C Disconnections: Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	[6L]
2.3	Two group C-C Disconnections: 1,2- 1,3- 1,4- 1,5- and 1,6- difunctionalized compounds, Diels-Alder reactions, α , β -unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annelation.	[6L]
Unit 3:	Electro-organic chemistry and Selected methods of Organic synthesis	[15L]
3.1	Electro-organic chemistry:	[7L]
3.1.1	Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.	
3.1.2	Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.	
3.1.3	Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.	
3.2	Selected Methods of Organic synthesis	[8L]
	Applications of the following in organic synthesis:	
3.2.1	Crown ethers, cryptands, micelles, cyclodextrins, catenanes.	
3.2.2	Organocatalysts: Proline, Imidazolidinone.	
3.2.3	Pd catalysed cycloaddition reactions: Stille reaction, Saegusa-Ito oxidation	

- to enones, Negishi coupling.
- 3.2.4 Use of Sc(OTf)₃ and Yb(OTf)₃ as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.
- Unit 4: Transition and rare earth metals in organic synthesis [15L]**
- 4.1 **Introduction to basic concepts:** 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion. [3L]
- 4.2 **Palladium in organic synthesis:** π -bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miyaura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms. [5L]
- 4.3 **Olefin metathesis** using Grubb's catalyst. [1L]
- 4.4 **Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis. [4L]
- 4.5 **Application of samarium iodide** including reduction of organic halides, aldehydes and ketones, α -functionalised carbonyl and nitro compounds. [1L]
- 4.6 **Application of Ce(IV)** in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent. [1L]

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- **Modern Methods of Organic Synthesis**, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
- **Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis**, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
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- **Organic Synthesis: The Disconnection Approach**, Stuart Warren, John Wiley & Sons, 2004
- **Name Reactions and Reagents in Organic Synthesis**, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
- **Name Reactions**, Jie Jack Lie, 3rd Edn., Springer
- **Organic Electrochemistry**, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: PSCHO403

Paper - III (Natural products and heterocyclic chemistry)

Unit 1:	Natural products-III	[15L]
1.1	Steroids: General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acids.	[5L]
1.2	Synthesis of 16-DPA from cholesterol and plant sapogenin.	[2L]
1.3	Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.	[5L]
1.4	Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.	[3L]
Unit 2:	Natural products-IV	[15L]
2.1	Vitamins: Classification, sources and biological importance of vitamin B ₁ , B ₂ , B ₆ , folic acid, B ₁₂ , C, D ₁ , E (α -tocopherol), K ₁ , K ₂ , H (β - biotin). Synthesis of the following: Vitamin A from β -ionone and bromoester moiety. Vitamin B ₁ including synthesis of pyrimidine and thiazole moieties Vitamin B ₂ from 3, 4-dimethylaniline and D(-)-ribose Vitamin B ₆ from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis) Vitamin E (α -tocopherol) from trimethylquinol and phytol bromide Vitamin K ₁ from 2-methyl-1, 4-naphthaquinone and phytol.	[5L]
2.2	Antibiotics: Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and β -nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected).	[6L]
2.3	Naturally occurring insecticides: Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.	[2L]
2.4	3.4 Terpenoids: Occurrence, classification, structure elucidation,	[2L]

stereochemistry, spectral data and synthesis of zingiberene .

Unit 3: Heterocyclic compounds-I [15L]

Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines.

Unit 4: Heterocyclic compounds-II [15L]

Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms). (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines. Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and acridines.

REFERENCES:

1. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssell, Apotekarsocieteten – Swedish Pharmaceutical Press.
2. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011.
3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
4. Chemistry of natural products, F. F. Bentley and F. R. Dollish, 1974
5. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.Ito Majori and S. Nozoo, Academic Press, 1974.
6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
7. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007.
8. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd., 1990.
9. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2nd edition, 1982.
10. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press, 1980.
11. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
12. An Introduction to the Chemistry of Heterocyclic Compounds, 2nd edition, B.M. Acheson, 1975.

13. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S.Davidson, J.B.Hobbs, D.V. Banthrope and J. B. Harborne, Longman,Essex, 1994.
14. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6th edition, Pearson.
15. Stereoselective Synthesis: A Practical Approach, M. Nogradi, Wiley-VCH, 1995.
16. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
17. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
18. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
19. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
20. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
21. Total. Synthesis of Longifolene, J. Am. Chem. Soc., E. J. Corey, M. Ohno, R. B. Mitra, and P. A. Vatakencherry. 1964, 86, 478.
22. Total. Synthesis of Longifolene, J. Am. Chem. Soc. 1961, 83, 1251.
- 23. The structure and total synthesis of 5-Vetivone, J. A. Marshall and P. C. Johnson, J. Org. Chem., 35, 192 (1970).**
- 24. Total synthesis of spirovetivanes, J. Am. Chem. Soc. 1967, 89, 2750.**
25. The Total Synthesis of Reserpine, Woodward, R. B.; Bader, F. E.; Bickel, H., Frey, A. J.; Kierstead, R. W. Tetrahedron 1958, 2, 1-57.
- 26. Total synthesis of Griseofulvin, Stork, G.; Tomasz, M. J. Am. Chem. Soc. 1962, 84, 310.**
- 27. Synthesis of (±)-4-demethoxydaunomycinone, A. V. Rama Rao , G. Venkatswamy , S. M. Javeed M. , V. H. Deshpande, B. Ramamohan Rao, J. Org. Chem., 1983, 48 (9), 1552.**
28. The Alkaloids, The fundamental Chemistry A biogenetic approach, Marcel Dekker Inc. New York, 1979.
29. Comprehensive Organic Chemistry by Barton and Ollis, Pergamon Press, Oxford, 1979.
30. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
31. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwood Limited, 1981.
32. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.
- 33. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons.**
34. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng,

Wiley Interscience.

35. Classics in Total Synthesis , K. C. Nicolaou and E. J. Sorensen, Weinheim: VCH, 1996.
36. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
37. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
38. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
39. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
40. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
41. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
42. Organic structures from spectra, [L. D. Field](#), [S. Sternhell](#), [John R. Kalman](#), Wiley, 4th ed., .2011
43. Introduction to spectroscopy, [Donald L. Pavia](#), [Gary M. Lampman](#), [George S. Kriz](#), James R. Vyvyan, 4th ed., 2009.
44. Organic spectroscopic structure determination: a problem-based learning approach [Douglass F. Taber](#), Oxford University Press, 17-Sep-2007.
45. Organic Spectroscopy: Principles And Applications, [Jag Mohan](#), Alpha Science International Ltd., 30-Mar-2004
46. Alkaloids, V.K. Ahluwalia, Ane Books Pvt.Ltd.
47. Biotransformations in Organic Chemistry, 5th Edition, Kurt Faber, Springer
48. Structure Determination of Organic Compounds, EPretsch, P. Buhlmann, C.Affolter, Springer

Course Code: PSCHOOC-I 404

Paper – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1:	[15L]
Introduction to Intellectual Property:	[2L]
Historical Perspective, Different types of IP, Importance of protecting IP.	
Patents:	[5L]
Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	
Industrial Designs:	[2L]

Definition, How to obtain, features, International design registration. [2L]
Copyrights:

Introduction, How to obtain, Differences from Patents. [2L]
Trade Marks:

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. [2L]
Geographical Indications:

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit 2: [15L]

Trade Secrets: [2L]

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: [2L]

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: [2L]

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): [5L]

- (i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement
- (ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.
- (iii) Berne Convention
- (iv) Budapest Treaty

(b) Paris Convention [6L]

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity.

Unit III: [15L]

Introduction to Cheminformatics: [5L]

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: [5L]

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: [5L]

Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Unit IV: [15L]

Applications:

Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.

REFERENCES:

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH
3. Gupta, S. P. *QSAR and Molecular Modeling*. Springer-Anamaya Pub.: New Delhi.

Course Code: PSCHOOC-II 404

PAPER – IV: RESEARCH METHODOLOGY

Unit 1: [15L]

Print: [5L]

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: [5L]

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: [5L]

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

Unit II: DATA ANALYSIS [15L]

The Investigative Approach:

Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.

Analysis and Presentation of Data:

Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.

Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING [15L]

SCIENTIFIC PAPERS

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.

Writing Scientific Papers:

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.

Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS

[15L]

Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

REFERENCES:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry*, 2nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistry and in general scientific data analysis* Cambridge University Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

Semester IV: Practicals Course code: PSCHO4P1

Two steps preparations

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenyl

indole.

- 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol.
- Cyclohexanone → cyclohexanone oxime → Caprolactum.
- Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone.
- 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid.
- o*-nitroaniline → *o*-phenylene diamine → Benzimidazole.
- Benzophenone → benzophenone oxime → benzanilide.
- o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
- Benzoin → benzil → benzoic acid.
- Phthalic acid → phthalimide → anthranilic acid.
- Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy coumarin.
- Anthracene → anthraquinone → anthrone.

(Minimum 8 experiments)

Note:

- Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
- Students are expected to purify the product by recrystallization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

Course code: PSCHO4P2

Session-I: Combined spectral identification: Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra).

A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring to any standard text-book/reference material etc

(Minimum 8 spectral analysis).

Session-II: Project evaluation

References for Practicals

- Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.
K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
- Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
- Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
- Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall

7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
8. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Edward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition, 2008, B.S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

②

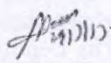
UNIVERSITY OF MUMBAI
No. UG/138 of 2017

CIRCULAR:-

A reference is invited to the Syllabi relating to the Master of Science (M.Sc) degree course, vide this office Circular No. UG/24 of 2013-14, dated 13th May, 2013 and the Head University Department of Chemistry and Principals of the affiliated Colleges in Science and the Directors / Heads of the recognized Institutions concerned are hereby informed that the recommendation made by Ad-hoc Board of Studies in Chemistry at its meeting held on 7th June, 2017, has been accepted by the Academic Council at its meeting held on 11th May, 2017 vide item No. 4.208 and that in accordance therewith, in revised syllabus as per the (CBCS) for M.Sc Part – I (Sem – I & II) (Chemistry). Which is available on the University's website (www.mu.ac.in) and that the same has been brought into force with effect from the academic year 2017-18.

MUMBAI – 400 032

31ST July, 2017


REGISTRAR

To,

The Head, University Department of Chemistry and the Principal of the affiliated Colleges in Science and the Head of Recognized Institutions concerned.

A.C/4.208/11.05.2017

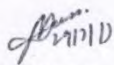
No. UG/138 -A of 2017

MUMBAI-400 032

31ST July, 2017

Copy forwarded with compliments for information to :-

- 1) The Co-ordinator, Faculty of Science,
- 2) The Offg. Director Board of Examinations and Evaluation,
- 3) The Chairman, Board of Studies in Chemistry.
- 4) The Director, Board of Students Development,
- 5) The Professor-cum-Director, Institute of Distance and Open Learning.
- 6) The Co-Ordinator, University Computerization Centre.


REGISTRAR

...PTO

AC: 11-05-2017

Item No. 4.208

UNIVERSITY OF MUMBAI

Syllabus for Approval

Sr. No.	Heading	Particulars
1	Title of Course	M.Sc. Chemistry Semester I and II
2	Eligibility for Admission	The B.Sc. degree examination of this university with chemistry 6 units or 3 units or degree of any other university recognized as equivalent thereto .
3	Passing marks	Minimum D Grade or equivalent minimum marks for passing at the Graduation level.
4	Ordinances/Regulations (if any)	
5	No. of Years/Semesters	One year/Two semester
6	Level	P.G. part-I
7	Pattern	Semester
8	Status	Revised
9	To be implemented from Academic year	2017-2018

Date: 05-5-2017

BoS Chairperson:

Signature:

Dr. Anil V. Karnik

Proposed Draft Syllabus For
M.Sc. Chemistry
Semester I and II
Choice Based Credit System
(To be implemented from the academic year, 2017-2018)

Semester – I

Paper I

Physical Chemistry: Course Code: PSCH 101

[60 L]

Unit - I

Thermodynamics-I [15]

- 1.1. State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants. **[8L]**
- 1.2. Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy. **[7L]**
[Ref 2 and 1,10,11,12 17]

Unit II

Quantum Chemistry: [15L]

- 2.1. Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.
- 2.2. Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.
- 2.3. Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation, Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation.
- 2.4. Application of quantum mechanics to the following systems:
 - a) Free particle, wave function and energy of a free particle.

- b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels.
- c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.
- [Ref 7, 8 and 9]

Unit III

Chemical Dynamics-I [15L]

3.1.Composite Reactions:

Recapitulation: Rate laws, Differential rate equations Consecutive reactions, Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.

3.2.Polymerization reactions: Kinetics of stepwise polymerization, Calculation of degree of polymerization for stepwise reaction. Kinetics of free radical chain polymerization, Kinetic chain length and estimation of average no .of monomer units in the polymer produced by chain polymerization.

3.3.Reaction in Gas Phase

Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.

[Ref. 2 and 15, 17, 18]

Unit IV

Electrochemistry [15L]

Recapitulation – basics of electrochemistry.

- 4.1.Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's extension to higher concentration (derivations are expected).
- 4.2.Electrolytic conductance and ionic interaction, relaxation effect,. Debye-Hückel-Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.

4.3. Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells
[Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]

4.4. Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme-catalysed oxidation of styrene. Goldman equation. (derivations are expected)

[Ref: 14 and 16, 17, 18]

[Note: Numerical and theoretical problems from each unit are expected]

References:

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7th Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2nd Edn., McMillan and Co. Ltd., London, 1962
7. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
8. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
9. R.K. Prasad, *Quantum Chemistry*, 2nd Edn., New Age International Publishers, 2000.
10. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
11. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
13. Ira N. Levine, *Quantum Chemistry*, 5th Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
14. Thomas Engel and Philip Reid, *Physical Chemistry*, 3rd Edn., Pearson Education Limited 2013.
15. D.N. Bajpai, *Advanced Physical Chemistry*, S. Chand 1st Edn., 1992.
16. **Bockris**, John O'M., **Reddy**, Amulya K.N., Gamboa-Aldeco, Maria E., *Modern Electrochemistry*, 2A, Plenum Publishers, 1998.
17. *Physical Chemistry* by Gurtu and Gurtu
18. *A Text book of Physical Chemistry* by K L Kapoor Vol 5 , 2nd Edn

Physical Chemistry Practical

Paper I

Course Code: PSCHP 101

Non – Instrumental:

1. To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperature.
2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of CaSO_4 at room temperature.
3. To investigate the reaction between acetone and iodine.
4. To study the variation in the solubility of Ca(OH)_2 in presence of NaOH and hence to determine the solubility product of Ca(OH)_2 at room temperature.
5. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

Instrumental:

1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
3. To determine pK_a values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.

References:

- 1 Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 2 Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edn., Longman Group Ltd., 1974.
- 3 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Paper II
Inorganic Chemistry: Course Code: PSCH 102
(60 L)

Unit I

Chemical Bonding: [15 L]

- 1.1 **Recapitulation of hybridization** Derivation of wave functions for sp , sp^2 , sp^3 orbital hybridization types considering only sigma bonding.
- 1.2 Discussion of involvement of d orbitals in various types of hybridizations. Concept of resonance, resonance energy derivation expected. Formal charge with examples.
- 1.3 Critical analysis of VBT.
- 1.4 Molecular Orbital Theory for diatomic species of First transition Series.
- 1.5 Molecular Orbital Theory for Polyatomic species considering σ bonding for SF_6 , CO_2 , B_2H_6 , I_3^- molecular species.
- 1.6 Weak forces of attraction: Hydrogen bonding – concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.

Unit-II

Molecular Symmetry and Group Theory: [15L]

- 2.1. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.
- 2.2. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.
- 2.3. Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups C_{2v} , C_{3v} and D_{2h} , structure of character tables.
- 2.4. Applications of Group Theory
 - (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in AB_n (Ammonia, CH_4) molecule.
 - (b) Determination of symmetry species for translations and rotations.
 - (c) Mulliken's notations for irreducible representations.
 - (d) Reduction of reducible representations using reduction formula.
 - (e) Group-subgroup relationships.
 - (f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.

Unit–III

Materials Chemistry and Nanomaterials: [15 L]

3.1 Solid State Chemistry

- 3.1.1. Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.
- 3.1.2. Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB₂ [fluorite (CaF₂) and anti-fluorite structures, rutile (TiO₂) structure and layer structure [cadmium chloride and iodide (CdCl₂, CdI₂)].
- 3.1.3. Methods of preparation for inorganic solids: Ceramic method, precursor method, sol-gel method (applications in Biosensors), microwave synthesis (discussion on principles, examples, merits and demerits are expected)

3.2 Nanomaterials

- 3.2.1. Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.
- 3.2.2. Applications in the field of semiconductors, solar cells

Unit - IV

Characterisation of Coordination compounds [15L]

- 4.1. Formation, thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.
- 4.2. Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as Δ , B, C, Nephelauxetic ratio.
- 4.3. Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.

References :

Unit I

1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
2. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2nd Ed., Academic Press, 1993.
3. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.
4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2nd Edition 2005.
5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure and Reactivity, 4th Ed., Harper Collins, 1993.
6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.

7. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.
8. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.
9. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.
10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
11. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.

Unit II

1. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.
2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1996.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.
5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.
6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.
7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

Unit III

1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-203-49635-3, Taylor & Francis Group, LLC.
2. Nanomaterials & Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
3. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.
5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.

6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.

Unit IV

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.
2. D. Banerjea ,Coordination Chemistry
3. Geary Coordination reviews
4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999,
6. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry*(3rd edn.), John Wiley & Sons (1994).

Inorganic Chemistry Practical

Paper II

Course Code: PSCHP 102

Inorganic Preparations (Synthesis and Characterization)

- 1) Bis-(tetraethylammonium) tetrachloro Cuprate (II) $(Et_4N)_2[CuCl_4]$
- 2) Bis-(tetraethylammonium) tetrachloro Nickelate (II) $(Et_4N)_2[NiCl_4]$
- 3) Bis-(tetraethylammonium) tetrachloro Cobaltate (II) $(Et_4N)_2[CoCl_4]$
(Any two from above preparations)
- 4) Tetrammine monocarbonato Cobalt (III) Nitrate $[Co(NH_3)_4CO_3]NO_3$
- 5) Bis (ethylenediammine) Copper (II) Sulphate $[Cu(en)_2]SO_4$
- 6) Hydronium dichloro bis(dimethylglyoximate) Cobaltate(III) $H[Co(dmgh)_2Cl_2]$

Instrumentation

- 1) Determination of equilibrium constant by Slope intercept method for Fe^{+3}/SCN^- system
- 2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.

Reference:

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

Paper III
Organic Chemistry: Course Code: PSCH 103
Lectures: 60 L

Unit I

Physical Organic Chemistry: (15 L)

- 1.1. Thermodynamic and kinetic requirements of a reaction:** rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity *vs* selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic *vs* thermodynamic control of organic reactions.
- 1.2. Determining mechanism of a reaction:** Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence.
- 1.3. Acids and Bases:** Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pK_a values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples.

[Reference Books: 1, 2, 3, 16]

Unit II

Nucleophilic substitution reactions and Aromaticity

2.1. Nucleophilic substitution reactions: (9 L)

- 2.1.1. Aliphatic nucleophilic substitution:** S_N1, S_N2, S_Nⁱ reactions, mixed S_N1 and S_N2 and SET mechanisms. S_N reactions involving NGP - participation by aryl rings, α- and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. S_NC_A, S_N1' and S_N2' reactions. S_N at sp² (vinylic) carbon.
- 2.1.2. Aromatic nucleophilic substitution:** S_NAr, S_N1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution.
- 2.1.3. Ester hydrolysis:** Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.

2.2. Aromaticity: (6 L)

- 2.2.1. Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.
- 2.2.2. Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's $(4n+2)$ and $4n$ rules.
- 2.2.3. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C_{60}).

[Reference Books: 4-15]

Unit-III

Stereochemistry: (15 L)

- 3.1. **Concept of Chirality:** Recognition of symmetry elements.
- 3.2. **Molecules with tri- and tetra-coordinate centers:** Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.
- 3.3. **Molecules with two or more chiral centers:** Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.
- 3.4. **Axial and planar chirality:** Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R,S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes.
- 3.5. **Prochirality:** Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiral centre, iii) a prochiral axis iv) a prochiral plane v) pro-pseudoasymmetric centre. Symbols for enantiotopic and diastereotopic faces.

[Reference Books: 6-8]

Unit-IV

Oxidation and Reduction: (15 L)

- 4.1. **Oxidation:** General mechanism, selectivity, and important applications of the following:

- 4.1.1. Dehydrogenation:** Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).
- 4.1.2. Oxidation of alcohols to aldehydes and ketones:** Chromium reagents such as $K_2Cr_2O_7/H_2SO_4$ (Jones reagent), CrO_3 -pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.
- 4.1.3. Oxidation involving C-C bonds cleavage:** Glycols using HIO_4 ; cycloalkanones using CrO_3 ; carbon-carbon double bond using ozone, $KMnO_4$, CrO_3 , $NaIO_4$ and OsO_4 ; aromatic rings using RuO_4 and $NaIO_4$.
- 4.1.4. Oxidation involving replacement of hydrogen by oxygen:** oxidation of CH_2 to CO by SeO_2 , oxidation of arylmethanes by CrO_2Cl_2 (Etard oxidation).
- 4.1.5. Oxidation of aldehydes and ketones:** with H_2O_2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)
- 4.2. Reduction:** General mechanism, selectivity, and important applications of the following reducing reagents:
- 4.2.1. Reduction of CO to CH_2 in aldehydes and ketones-** Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification.
- 4.2.2. Metal hydride reduction:** Boron reagents ($NaBH_4$, $NaCNBH_3$, diborane, 9-BBN, $Na(OAc)_3BH$, aluminium reagents ($LiAlH_4$, DIBAL-H, Red Al, L and K- selectrides).
- 4.2.3.** NH_2NH_2 (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzsch dihydropyridine).
- 4.2.4. Dissolving metal reductions:** using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH_3 mediated reduction (Birch reduction) of aromatic compounds and acetylenes.

[Reference Books: 17, 18, 14]

Reference Books:

1. Physical Organic Chemistry, Neil Isaacs
2. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
3. Comprehensive Organic chemistry, Barton and Ollis, Vol 1
4. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
6. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
7. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Manden, Wiley.

8. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
9. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
10. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
13. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
14. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
15. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
16. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
17. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
18. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, Pragati Prakashan.

**Organic Chemistry Practical
Paper III
Course Code: PSCHP 103**

One step preparations (1.0 g scale)

1. Bromobenzene to p-nitrobromobenzene
2. Anthracene to anthraquinone
3. Benzoin to benzil
4. Anthracene to Anthracene maleic anhydride adduct
5. 2-Naphthol to BINOL
6. p-Benzoquinone to 1,2,4-triacetoxybenzene
7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
8. *o*-Phenylenediamine to 2-methylbenzimidazole
9. *o*-Phenylenediamine to 2,3-diphenylquinoxaline
10. Urea and benzil to 5,5-diphenylhydantoin

Learning points:

1. Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.

2. Purify the product by crystallization. Formation and purity of the product should be checked by TLC
3. Report mass and melting point of the purified product.

Paper IV
Analytical Chemistry: Course Code: PSCH 104
Lectures: 60 L

Unit - I

1.1 Language of Analytical Chemistry [8 L]

1.1.1 Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol)

1.1.2 An overview of analytical methods, types of instrumental methods, instruments for analysis, data domains, electrical and non-electrical domains, detectors, transducers and sensors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range.

1.1.3 Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors. **1.1.4** Quantitative methods of analysis: calibration curve, standard addition and internal standard method.

1.2 Quality in Analytical Chemistry: [7 L]

1.2.1 Quality Management System (QMS):

Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.

1.2.2 Safety in Laboratories:

Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts).

1.2.3 Accreditations:

Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, Agmark)

1.2.4 Good Laboratory Practices (GLP)

Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score

Unit- II

Calculations based on Chemical Principles [15 L]

The following topics are to be covered in the form of numerical problems only.

- a. Concentration of a solution based on volume and mass units.
- b. Calculations of ppm, ppb and dilution of the solutions, concept of mmol.

- c. Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.
- d. Solubility and solubility equilibria, effect of presence of common ion.
- e. Calculations of pH of acids, bases, acidic and basic buffers.
- f. Concept of formation constants, stability and instability constants, stepwise formation constants.
- g. Oxidation number, rules for assigning oxidation number, redox reaction in term of oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a solution of a oxidizing / reducing agent and its relationship with molarity).

Unit III

Optical Methods [15 L]

3.1 Recapitulation and FT Technique [3 L]

3.1.1 Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.

3.1.2 Laser as a source of radiation, Fibre optics

3.1.3 Introduction of Fourier Transform

3.2 Molecular Ultraviolet and Visible Spectroscopy [6 L]

NUMERICALS ARE EXPECTED

3.2.1 Derivation of Beer- Lambert's Law and its limitations, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents.

Applications of Ultraviolet and Visible spectroscopy:

- 1) On charge transfer absorption
- 2) Simultaneous spectroscopy
- 3) Derivative Spectroscopy

3.2.2 Dual spectrometry – Introduction, Principle, Instrumentation and Applications

3.3 Infrared Absorption Spectroscopy [6 L]

3.3.1 Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument **05 L**

3.3.2 FTIR and its advantages

3.3.3 Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR

3.3.4 Introduction and basic principles of diffuse reflectance spectroscopy.

Unit - IV

4.1 Thermal Methods: [9 L]

4.1.1 Introduction, Recapitulation of types of thermal methods, comparison between TGA and DTA.

4.1.2 Differential Scanning Calorimetry- Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure).

4.1.3 Applications - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.

4.2 Automation in chemical analysis: [6 L]

Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators.

References

Unit I

1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education
2. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th Edition, Ch: 1.
3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.
4. Undergraduate Instrumental Analysis, 6th Edition, J W Robinson, Marcel Dekker, Ch:1.
5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 & 4) (Free download).
6. Quality in the Analytical Laboratory, Elizabeth Pichard, Wiley India, Ch: 5, Ch: 6 & Ch: 7.
7. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
8. Quality in Totality: A Manager's Guide To TQM and ISO 9000, Parag Diwan, Deep & Deep Publications, 1st Edition, 2000.
9. Quality Control and Total Quality Management - P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management - Bester field - Pearson Education, Ch:5.
10. Industrial Hygiene and Chemical Safety, M H Fulekar, Ch:9, Ch:11 & Ch:15.
11. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
12. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
13. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.
14. Klimisch, HJ; Andrae, M; Tillmann, U (1997). "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data". doi:10.1006/rtp.1996.1076. PMID 9056496.

Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, Mc Graw Hill international Editions, Chapter 11,15,16,21,22

Unit III

1. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Harcourt Asia Publisher. Chapter 6, 7.
2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6th Edition, CBS Publisher. Chapter 2.
3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.
4. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Harcourt Asia Publisher. Chapter 13, 14.
5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6th Edition, CBS Publisher. Chapter 2.
6. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 5.
7. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5th Edition, McGraw Hill Publisher, Chapter 3.
8. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.
9. A. J. Somnessa, The effect of temperature on the visible absorption band of iodine in several solvents, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525-528.
10. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Harcourt Asia Publisher. Chapter 16, 17.
11. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 12
12. Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. Theophanides Theophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech,(open access)

Unit IV

1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27
2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications
3. Instrumental methods of analysis, 7th Edition, Willard, Merrit, Dean: Chapter 25
4. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 31
5. Quantitative Chemical Analysis, 6th Edition, Vogel: Chapter 12
6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Kenneth H. Tonge
7. Instrumental methods of analysis, 7th Edition, Willard, Merrit, Dean: Chapter 26
8. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 33
9. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 28

Analytical Chemistry Practical

Paper IV

Course Code: PSCHP 104

1. To carry out assay of the sodium chloride injection by Volhard's method.
Statistical method.
2. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3. To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
4. To determine the breakthrough capacity of a cation exchange resin.
5. To determine the lead and tin content of a solder alloy by titration with EDTA.
6. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
7. To determine number of nitro groups in the given compound using TiCl_3 .

References:

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company,Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part-II,4th Ed.,A Wiley Interscience Publication,New York,1978.

Semester – II

Paper I

Physical Chemistry: Course Code: PSCH 201

[60 L]

Unit I

Chemical Thermodynamics II [15 L]

- 1.1. Fugacity of real gases, Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.
- 1.2. **Real solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation.
- 1.3. **Thermodynamics of surfaces**, Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).
- 1.4. Bioenergetics : standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Unit II

Quantum Chemistry II [15 L]

- 2.1. Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the ϕ equation, wavefunction, quantum number, the θ equation, wave function, quantization of rotational energy, spherical harmonics.
- 2.2. Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the R the θ * and the ϕ equations, solution of the equation, introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, distances and energies in atomic units, radial and angular plots., points of maximum probability, expressions for the total wave function for 1s,2s, 2p and 3d orbitals of hydrogen.
- 2.3. Application of the Schrödinger equation to two electron system, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate solution of the Schrödinger wave equation.
- 2.4. Hückel Molecular Orbitals theory for ethylene , 1,3-butadiene and benzene. (*Derivation expected*)

Unit III

Chemical Kinetics and Molecular Reaction Dynamics [15 L]

- 3.1. **Elementary Reactions in Solution:-** Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action
- 3.2. **Kinetics of reactions catalyzed by enzymes** -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses.
- 3.3. **Inhibition of Enzyme action:** Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.
- 3.4. **Kinetics of reactions in the Solid State:-** Factors affecting reactions in solids
Rate laws for reactions in solid: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies.
(Ref: 7 and 2)

Unit IV

Solid State Chemistry and Phase Equilibria [15 L]

4.1 : Solid State Chemistry

4.1.1. **Recapitulation:** Structures and Defects in solids.

Types of Defects and Stoichiometry

- a) Zero dimensional (point) Defects
- b) One dimensional (line) Defects
- c) Two dimensional (Planar) Defects
- d) Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it)

(Ref: 17, 18 and 19)

4.2 Phase equilibria

4.2.1. **Recapitulation:** Introduction and definition of terms involved in phase rule. Thermodynamic derivation of Gibbs Phase rule.

4.2.2. **Two component system:**

- a) Solid –Gas System : Hydrate formation, Amino compound formation
- b) Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point . (with suitable examples)

4.2.3. **Three component system**

Type-I : Formation of one pair of partially miscible liquids

Type-II: Formation of two pairs of partially miscible liquids

Type-III: Formation of three pairs of partially miscible liquids

(Ref: 4, 6, 11, 12 ,13,16, 24)

References

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7th Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2nd Edn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007.
8. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
9. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
10. R.K. Prasad, *Quantum Chemistry*, 2nd Edn., New Age International Publishers, 2000.
11. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
12. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
14. Ira N. Levine, *Quantum Chemistry*, 5th Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
15. Thomas Engel and Philip Reid, *Physical Chemistry*, 3rd Edn., Pearson Education Limited 2013.
16. D.N. Bajpai, *Advanced Physical Chemistry*, S. Chand 1st Edn., 1992.
17. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart & Elaine A. Moore, Taylor & Francis, 2010.
18. The Physics and 'Chemistry of Solids, Stephen Elliott, Willey India, 2010
19. Principles of the Solid State, H.V. Keer, New Age International Publishers, 2011.
20. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
21. Principles of physical Chemistry , Marrown and Prutton 5th edition
22. Essentials of Physical Chemistry , Arun Bahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
23. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
24. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011
25. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

Physical Chemistry Practical

Paper I

Course Code: PSCHP 201

Non – instrumental:

1. Polar plots of atomic orbitals such as $1s$, $2p_x$ and $3d_{z^2}$ orbitals by using angular part of hydrogen atom wave functions.
2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.
3. To study phase diagram of three component system water – chloroform /toluene - acetic acid.
4. To determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.

Instrumental:

1. To determine the formula of silver ammonia complex by potentiometric method.
2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
3. To determine Hammett constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by pH measurement.
4. To determine the Michaelis – Menten's constant value (K_m) of the enzyme Beta Amylase spectrophotometrically.

References

- 4 Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 5 Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edn., Longman Group Ltd., 1974.
- 6 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Semester II

Paper II

Inorganic Chemistry: Course Code: PSCH 202

Unit I

Inorganic Reaction Mechanism: [15 L]

- 1.1 Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods).
- 1.2 Ligand substitution reactions of:
 - a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method)
 - b) Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.
- 1.3 Redox reactions: inner and outer sphere mechanisms, complimentary and non-complimentary reactions.
- 1.4 Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)

Unit II

Organometallic Chemistry of Transition metals: [15 L]

- 2.1. Eighteen and sixteen electron rule and electron counting with examples.
- 2.2. Preparation and properties of the following compounds
 - (a) Alkyl and aryl derivatives of Pd and Pt complexes
 - (b) Carbenes and carbynes of Cr, Mo and W
 - (c) Alkene derivatives of Pd and Pt
 - (d) Alkyne derivatives of Pd and Pt
 - (e) Allyl derivatives of nickel
 - (f) Sandwich compounds of Fe, Cr and Half Sandwich compounds of Cr, Mo.
- 2.3 Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:

Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0)
[Pt(PPh₃)₂(HC≡CPh)₂], diallylnickel(II), ferrocene and bis(arene)chromium(0),
tricarbonyl (η^2 -butadiene) iron(0).

Unit III

Environmental Chemistry:[15 L]

- 3.1. **Conception of Heavy Metals:** Critical discussion on heavy metals

- 3.2. Toxicity of metallic species:** Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.
- 3.3. Case Studies:**
- (a) Itai-itai disease for Cadmium toxicity,
 - (b) Arsenic Poisoning in the Indo-Bangladesh region.
- 3.4. Interaction of radiation in context with the environment:** Sources and biological implication of radioactive materials. Effect of low level radiation on cells- Its applications in diagnosis and treatment, Effect of radiation on cell proliferation and cancer.

Unit IV

Bioinorganic Chemistry:[15 L]

- 4.1. Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and it's implications.
- 4.2. Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases- structure of the metal center and mechanism of oxygen activation by these enzymes.
- 4.3. Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site
- 4.4. Nitrogen fixation-nitrogenase, hydrogenases
- 4.5. Metal ion transport and storage: Ionophores, transferrin, ferritin and metallothionins
- 4.6. Medicinal applications of cis-platin and related compounds

References

Unit I

- 1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th Ed., Oxford University Press, 2010.
- 2. D. Banerjee, Coordination Chemistry, Tata McGraw Hill, 1993.
- 3. W. H. Malik, G. D./ Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8th Ed., S. Chand & Company Ltd.
- 4. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
- 5. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002
- 6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12th Edition, Goel publishing house, 2012.

7. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
8. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.
9. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.
10. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed., Oxford University Press 2008.

Unit II

1. D. Banerjea, Coordination chemistry. Tata McGraw Hill, New Delhi, 1993.
2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, New Age International Pvt Ltd, 2000.
3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.
4. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons. 1983.
5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

Unit III

1. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
2. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,
3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
4. Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.
5. Fundamentals of Environmental and Toxicological Chemistry 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor & Francis Group, 2013.
6. Living in the Environment 17th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-538-49414-X, Brooks/Cole, Cengage Learning, 2011
7. Poisoning and Toxicology Handbook, Jerrold B. Leikin, Frank P. Paloucek, ISBN: 1-4200-4479-6, Informa Healthcare USA, Inc.
8. Casarett and Doull's Toxicology- The Basic Science of Poisons 6th edition, McGraw-Hill, 2001.

Unit IV

1. R. W. Hay, *Bioinorganic Chemistry*, Ellis Harwood, England, 1984.
2. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.

3. J. A. Cowan, *Inorganic Biochemistry-An introduction*, VCH Publication, 1993.
4. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Publications, Mill Valley, California, 1994.
5. G.N. Mukherjee and A. Das, *Elements of Bioinorganic Chemistry*, Dhuri & Sons, Calcutta, 1988.
6. J.Chem. Educ. (Special issue), Nov, 1985.
7. E.Frienden, J.Chem. Educ., 1985, 62.
8. Robert R.Crechton, *Biological Inorganic Chemistry – An Introduction*, Elsevier
9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.
10. JM. D. Yudkin and R. E. Offord *A Guidebook to Biochemistry*, Cambridge University Press, 1980.

Inorganic Chemistry Practical

Paper II

Course Code: PSCHP 202

Ores and Alloys

- 1) Analysis of Devarda's alloy
- 2) Analysis of Cu – Ni alloy
- 3) Analysis of Tin Solder alloy
- 4) Analysis of Limestone.

Instrumentation

- 1) Estimation of Copper using Iodometric method Potentiometrically.
- 2) Estimation of Fe^{+3} solution using Ce(IV) ions Potentiometrically

Reference:

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

Paper III

Organic Chemistry: Course Code: PSCH 203

Lectures 60 L

Unit-I

1.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)

- 1.1.1. Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.
- 1.1.2. Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.
- 1.1.3. Alkylation of aldehydes, ketones, esters, amides and nitriles.
- 1.1.4. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.
- 1.1.5. Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).

1.2. Reaction of carbon nucleophiles with carbonyl groups: (8 L)

- 1.2.1. Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation.
- 1.2.2. Addition reactions with amines and iminium ions; Mannich reaction.
- 1.2.3. Amine catalyzed condensation reaction: Knoevenagel reaction.
- 1.2.4. Acylation of carbanions.

[Reference Books: 1-11]

Unit II

Reactions and Rearrangements: (15 L)

Mechanisms, stereochemistry (if applicable) and applications of the following:

- 2.1. **Reactions:** Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.
- 2.2. **Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.
- 2.3. **Cationic rearrangements:** Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.
- 2.4. **Anionic rearrangements:** Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Payne.

[Reference Books: 19-22]

Unit-III

3.1. Introduction to Molecular Orbital Theory for Organic Chemistry: (7 L)

3.1.1. Molecular orbitals: Formation of σ - and π -MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of π -MOs

3.1.2. Introduction to FMOs: HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO (π and π^* orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles. Concept of 'donor-acceptor' interactions in nucleophilic addition reactions on formaldehyde. Connection of this HOMO-LUMO interaction with 'curved arrows' used in reaction mechanisms. The concept of hardness and softness and its application to electrophiles and nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis of MOs.

3.1.3. Application of FMO concepts in (a) S_N^2 reaction, (b) Lewis acid base adducts (BF_3-NH_3 complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde.

3.2. Applications of UV and IR spectroscopy: (8 L)

3.2.1. Ultraviolet spectroscopy: Recapitulation, UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents).

3.2.2. Infrared spectroscopy: Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.

Unit-IV

NMR spectroscopy and Mass spectrometry (15 L)

- 4.1. Proton magnetic resonance spectroscopy:** Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei as in alcohols, phenols, enols, carboxylic acids, amines, amides. Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic). First order spectra, Karplus equation.
- 4.2. ^{13}C NMR spectroscopy:** Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons.
- 4.3. Mass spectrometry:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.
- 4.4.** Structure determination involving individual or combined use of the above spectral techniques.

[Reference Books: 13-18]

References:

1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.
3. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
4. Organic Chemistry, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7th Edition)
5. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
6. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
7. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
8. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
10. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
11. Mechanism in Organic Chemistry, Peter Sykes, 6th

12. Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley
13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
15. Organic Spectroscopy, William Kemp, W.H. Freeman & Company.
16. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.
17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.
18. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
19. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parasher, Alpha Science International, 2011.
20. Reactions, Rearrangements and Reagents by S. N. Sanyal
21. Name Reactions, Jie Jack Li, Springer
22. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Eller, and F.G. Favalaro, John Wiley & Sons.

**Organic Chemistry Practical
Paper III
Course Code: PSCHP 203**

Separation of Binary mixture using micro-scale technique

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component.
The following types are expected:
 - (i) Water soluble/water insoluble solid and water insoluble solid,
 - (ii) Non-volatile liquid-Non-volatile liquid (chemical separation)
 - (iii) Water-insoluble solid-Non-volatile liquid.

Minimum three mixtures from each type and a total of ten mixtures are expected.

Reference:

1. Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
2. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
3. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)
4. Practical Organic Chemistry by Mann and Saunders.
5. Advance Practical Organic Chemistry, N.K. Vishnoi, Vikas Publication

Paper IV

Analytical Chemistry: Course Code: PSCH 104

[60 L]

Unit I

Chromatography [15 L]

- 1.1 Recapitulation of basic concepts in chromatography:** Classification of chromatographic methods, requirements of an ideal detector, types of detectors in LC and GC, comparative account of detectors with reference to their applications (LC and GC respectively), qualitative and quantitative analysis. [2 L]
- 1.2** Concept of plate and rate theories in chromatography: efficiency, resolution, selectivity and separation capability. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions. [5 L]
- 1.3 Gas Chromatography:** Instrumentation of GC with special reference to sample injection systems – split/splitless, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications. [3 L]
- 1.4 High Performance Liquid Chromatography (HPLC):** Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns). Diode array type and fluorescence detector, Applications of HPLC. Chiral and ion chromatography. [5 L]

Unit II

- 2.1 X-ray spectroscopy:** principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy. [4 L]
- 2.2 Mass spectrometry:** recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications. [6 L]
- 2.3 Radioanalytical Methods** – recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications. [5 L]

Unit III

3.1 Surface Analytical Techniques – [9 L]

Introduction, Principle, Instrumentation and Applications of:

- 3.1.1** Scanning Electron Microscopy (SEM)
- 3.1.2** Scanning Tunneling Microscopy (STM)
- 3.1.3** Transmission Electron Microscopy (TEM)
- 3.1.4** Electron Spectroscopy (ESCA and Auger)

3.2 Atomic Spectroscopy [6 L]

3.2.1 Advantages and Limitations of AAS

3.2.2 Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.

Unit IV

Electroanalytical Methods (Numericals are Expected)

4.1 Ion selective potentiometry and Polarography: [10 L]

Ion selective electrodes and their applications (solid state, precipitate, liquid –liquid, enzyme and gas sensing electrodes), ion selective field effect transistors, biocatalytic membrane electrodes and enzyme based biosensors.

Polarography: Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves.

4.2 Electrogravimetry: Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications.[3 L]

4.3 Coulometry: Introduction, principle, instrumentation, coulometry at controlled potential and controlled current [2 L]

References:

Unit I

1. Instrumental Analysis, Skoog, Holler & Crouch
2. HPLC Practical and Industrial Applications, 2 nd Ed., Joel K. Swadesh, CRC Press

Unit II

1. Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)
2. Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy
3. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th Edition, Ch: 12
4. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th Edition, Ch: 20

Unit III

1. Instrumental Analysis by Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
2. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM
3. Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)
4. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.

5. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, New York, 1993.
6. 5. Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer
7. Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York
8. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
9. Instrumental Analysis by Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition (2003), ISBN10: 8131505421, ISBN-13: 978-8131505427

Unit IV

1. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th Edition, Harcourt College Publishers, 1998. Chapters - 23, 24, 25.
2. Analytical Chemistry Principles – John H Kennedy, 2nd edition, Saunders College Publishing (1990).
3. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
4. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
5. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
6. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.

Analytical Chemistry Practical

Paper IV

Course Code: PSCHP 204

1. To determine percentage purity of sodium carbonate in washing soda pH metrically.
2. To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
3. To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non aqueous medium using glass calomel system potentiometrically.
4. To determine the amount of nitrite present in the given water sample colorimetrically.
5. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
6. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
7. To determine the percentage composition of HCl and H₂SO₄ on weight basis in a mixture of two by conductometric titration with NaOH and BaCl₂.

8. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

References

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company, Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part-II, 4th Ed.,A Wiley Interscience Publication,New York,1978

Practical Examination

Practical examination of each paper for 50 marks will be held for three and half hours

Practical	40M
Journal	5M
Viva-voce	5M
Total	50M

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