

UNIVERSITY OF MUMBAI

No. UG/85 of 2018-19

CIRCULAR:-

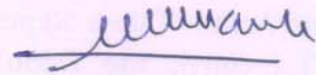
Attention of the Principals of the affiliated Colleges, the Head University Departments and Directors of the recognized Institutions in Science & Technology Faculty is invited to this office Circular Nos. UG/226 of 2006, dated 29th June, 2006 relating to syllabus of the Master of Science (M.Sc.) degree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

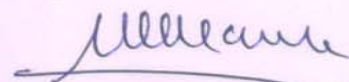
No. UG/ 85 -A of 2018

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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- Carey and Richard J. Sundberg, Springer.
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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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- **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.

Trade Marks: [2L]

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: [2L]

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.

UNIVERSITY OF MUMBAI

No. UG/88 of 2018-19

CIRCULAR:-

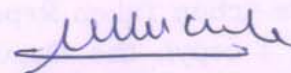
Attention of the Principals of the affiliated Colleges, the Head University Departments and Directors of the recognized Institutions in Science & Technology Faculty is invited to this office Circular Nos. UG/226 of 2006, dated 29th June, 2006 relating to syllabus of the Master of Science (M.Sc.) degree 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. 4.74 and that in accordance therewith, the revised syllabus as per the (CBCS) for the M.Sc. in Inorganic 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./4.74/14/06/2018

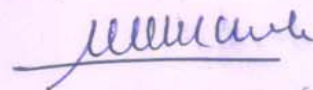
No. UG/ 88 -A of 2018

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

M.Sc. INORGANIC CHEMISTRY

SEMESTER III

Course Code	Unit	Topics
		(Numericals and word problems wherever possible.)
PSCHI 301		1. Chemistry of Inorganic Solids
	I	1.1 Descriptive Crystal Chemistry(15 L)
		(a) Simple structures
		Structures of AB type compounds (PbO and CuO), AB₂ type (β cristobalite, CaC ₂ and Cs ₂ O), A₂B₃ type (Cr ₂ O ₃ and Bi ₂ O ₃), AB₃ (ReO ₃ , Li ₃ N), ABO₃ type, relation between ReO ₃ and perovskite BaTiO ₃ and its polymorphic forms, Oxide bronzes, ilmenite structure, AB₂O₄ type, normal, inverse, and random spinel structures.
		(b) Linked Polyhedra
		(i) Corner sharing: tetrahedral structure (Silicates) and octahedral structure (ReO ₃) and rotation of ReO ₃ resulting in VF ₃ , RhF ₃ and calcite type structures. (ii) Edge sharing: tetrahedral structures (SiS ₂) and octahedral structures (BiI ₃ and AlCl ₃). pyrochlores, octahedral tunnel structures and lamellar structures
	II	1.2 Imperfection in crystals and Non-Stoichiometry (15 Lectures)
		(a) Point defects: Point defects in metals and ionic Crystal – Frenkel defect and Schottky defect. Thermodynamics formation of these defects (mathematical derivation to find defect concentration); Defects in non-Stoichiometric compounds, colour centres.
		(b) Line defects: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids.
		(c) Surface Defects: Grain Boundary and Stacking Fault. Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom Defects.
	1.3 Methods of Preparations (15 Lectures)	
	(a) Methods of Synthesis: Chemical Method, High Pressure Method, Arc Technique and Skull Method (with examples).	
III		(b) Different methods for single crystal growth:
		(i) Crystal Growth from Melt–: Bridgman and Stockbargar, Czochralski and Vernuil methods. (ii) Crystal growth from liquid solution: Flux growth and temperature gradient methods (iii) Crystal growth from vapor phase: – Epitaxial growth methods.
		(c) Thin film preparation: Physical and Chemical methods.
		(d) Solid Solutions: Formation of Substitutional, Interstitial and Complex Solid Solutions; Mechanistic Approach; Study of Solid solutions by X-ray

		Powder Diffraction and Density Measurement.
	IV	1.4 Behaviour of Inorganic Solids (15 Lectures) (a) Diffusion in Solids: Fick's Laws of Diffusion; Kirkendal Effect; Wagner mechanism, Diffusion and Ionic Conductivity; Applications of Diffusion in Carburizing and non-Carburizing Processes in Steel Making.
		(b) Solid state reactions: General principles and factors influencing reactions of solids, Reactivity of solids.
		(c) Liquid Crystals: Introduction and classification of thermotropic liquid crystals, Polymorphism in liquid crystal, Properties and applications of liquid crystals.
		<u>REFERENCE BOOKS</u>
		<ol style="list-style-type: none"> 1. L. E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005. 2. A.R. West, Solid State Chemistry and Its Applications, John Wiley & sons, 1987. 3. C.N.R. Rao and J.Gopalkrishnan New Directions in Solid State Chemistry, 2nd Ed., Cambridge University Press. 1997 4. L.V. Azaroff, Introduction to solids, Tata-McGraw Hill Book Co. New Delhi, 1977. 5. D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed. Wiley and sons, New York, 1966. 6. J.M. Hollas, Symmetry in Molecules, Chapman and Hall Ltd., 1972. 7. Reboert L carter, Molecular Symmetry and Group Hohn Wiley and Sons, New York, 1988. 8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993. 9. R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.. 10. H.V.Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993. Gary L.Miessler and Donald A.Tarr, Inorganic Chemistry, 3rd edition, Pearson Education, Inc., 2004. 11. D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996. 12. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press, N.Y. (1966)
		2. Bioinorganic and Coordination Chemistry.
PSCHI 302	I	2.1 Bioinorganic Chemistry(15 Lectures) (i)Coordination geometry of the metal ion and functions. (ii)Zn in biological systems: Carbonic anhydrase, protolytic enzymes, e.g. carboxy peptidase, Zinc finger.

		(iii) Role of metal ions in biological electron transfer processes: iron sulphur proteins, (iv) Less common ions in biology e.g. Mn (arginase; structure and reactivity), Ni (urease ; structure and reactivity) (v) Biomineralization
	II	2.2 Reactivity of Chemical Species –I (15 Lectures) 2.2.1 Recapitulation of the definition of Lewis acids and bases, Classification of Lewis acids and bases based on frontier Molecular orbital topology, Reactivity matrix of Lewis acids and bases. 2.2.2 Group Characteristic of Lewis acids (Gp-1,13-17). 2.2.3 Pauling rules to determine the strength of oxoacids; classification and Structural anomalies.
	III	2.3 Reactivity of Chemical Species –II (15 Lectures) 2.3.1 Pourbaix Diagrams. 2.3.2 Amphoteric behavior, Periodic trends in amphoteric properties of p-block and d-block elements 2.3.3 Oxoanions and Oxocations. 2.3.4 Measures of hardness and Softness of Acids and Bases, Drago-wayland equations 2.3.5 Applications of acid-base Chemistry: Super acids and Super bases, heterogeneous acid-base reactions.
	IV	2.4 Structure, Bonding, and Stereochemistry of Coordination Compounds (15 Lectures) (a) Structure and Bonding. i) Molecular Orbital Theory for Complexes with Coordination Number 4 and 5 for the central ion (sigma as well as Pi bonding) (ii) Angular Overlap Model for octahedral and tetrahedral complexes for sigma and pi bond. (b) Stereochemistry of Coordination Compounds. (i) Chirality and Fluxionality of Coordination Compounds with Higher Coordination Numbers. (ii) Geometries of Coordination compounds from Coordination number 6 to 9.
		<u>REFERENCES:</u> 1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., New Delhi; 2002. 2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3 rd edition. 3. James E. Huheey, Inorganic Chemistry, 3 rd edition, Harper &

		<p>Row, Publishers, Asia, Pte Ltd., 1983.</p> <ol style="list-style-type: none"> 4. W.W.Porterfield, Inorganic Chemistry-An Unified Approach, Academic press(1993); 5. D.F.Shriver, P.W.Atkins and C.H. Langford, Inorganic Chemistry, 3rd edition Oxford University Press, 1999. 6. Asim K.Das, Fundamental Concepts of Inorganic Chemistry, (Volumes-I, II and III) CBS Pub.(2000) 7. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, Pergamon, 1984. 8. J.M.Hollas, Symmetry in Chemistry, Chapmanad Hall Ltd., NY, 1972.\ 9. F.A.Cotton, Chemical Applications of Group Theory, 2nd edition, Wiley Eastern Ltd., New Delhi , 1976 10. C.J.Ballhausen and H.B.Gray, Molecular Orbital Theory, MCGraw-Hill, New York, 1965. 11. H. Sisler, Chemistry in Non-aqueous Solvents: New York Reinhold Publ. 1965. 12. . J.J. Lagowski, The Chemistry of Non-aqueous Solvents, Academic press, New york and London. 13. . C.M. Day and Joel Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt.Ltd., 1985. 14. L.E.Orgel, An Introduction to Ligand Field Theory , Methuen & Co.Ltd., London, 1960. 15. F.Basolo and R.G.Pearson, Mechanisms of Inorganic Reactions, Wiley, New York, 1967. 16. . J.D.Lee, Concise Inorganic Chemistry, 5th ed., Blackwell ScienceLtd., 2005. 17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New york, 1988. 18. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2nd edition, John Wiley & sons, Inc., New York, 1992. 19. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry, Prentice-Hall, (1997). 20. . R.C.Mehrotra and A.Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt.Ltd., 2000. 21. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983. 22. James E.Huheey, Inoganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972). 23. . F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999. 24. F.A. Cotton and R.A.Walton, Multiple Bonds between MetalAtoms, 2nd edition, claranden Press, Oxford, 1993. 25. P.L. Soni, Vandana Soni ,Ane Books Pvt.,Ltd
		3. Spectral Methods in Inorganic Chemistry
I		3.1 Diffraction Methods –I (15 Lectures) X-Ray Diffraction: Bragg Condition; Miller

PSCHI 303		Indices; Laue Method; Bragg Method; Debye Scherrer Method of X-Ray Structural Analysis of Crystals.	
	II	3.2 Diffraction Methods –II (15 Lectures) (a) Electron Diffraction: Scattering of electrons, Scattering Intensity versus Scattering Angle, Weirl Measurement Technique, Elucidation of Structures of Simple gas Phase Molecules. (b) Neutron Diffraction: Scattering of Neutrons: Scattering of neutrons by Solids and Liquids, Magnetic Scattering, Measurement Technique.	
	III	3.3 Electron Spin Resonance Spectroscopy (15 Lectures) (a) Electron behaviour, interaction between electron spin and magnetic field. (b) Instrumentation : Source, Sample cavity. Magnet and Modulation coils, Microwave Bridge, Sensitivity. (c) Relaxation processes and Line width in ESR transitions: (i) ESR relaxation and chemical bonding. (ii) Interaction between nuclear spin and electron spin (hyperfine coupling) (iii) Spin polarization for atoms and transition metal ions, (iv) Spin-orbit coupling and significance of gtensors, (v) Application to transition metal complexes (having one unpaired electron)	
	3.4 Mossbauer Spectroscopy (15 Lectures)		
IV	Mössbauer Spectroscopy: 3.4.1 Basic principle, recoil energy and Doppler shift. 3.4.2 Instrumentation: sources and absorber; motion devices, detection, reference substances and calibration, 3.4.3 Isomer shift, quadrupole interaction, magnetic interaction, electronegativity and chemical shift. 3.4.4 Applications: <i>Iron compounds</i> - low spin and high spin Fe(II) and Fe(III) compounds and complexes, effect of pi-bonding, mono and poly nuclear Iron complexes, spinel oxides and iron-sulphur proteins; <i>Tin compounds</i> - tin halides and tin oxides, organotin compounds; <i>Iodine compounds</i> - I ₂ and alkali metal iodide compounds.		
		<u>REFERENCES:</u> 1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis Fifth edition, (1996), ELBS Publication. Chapter 2, 3, 11. 2. W.H. Zachariasen. Theory of X-Ray Diffraction in Crystals. JohnWiley. New York. 1946.	

		<ol style="list-style-type: none"> 3. B.D. Cality,, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954. 4. R. Reaching, Electron Diffraction, Methuen and Co. London. 1936 5. May and Leopold, An Introduction to Mossbauer Spectroscopy, Plenum, New York, 1971. 6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, C.B.S. Publishers and Distributors, New Delhi, 1986. 7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press, Oxford, 1995. 8. Reverts John D., Nuclear Magnetic Resonance, McGraw Hill, New York, 1959. 9. . H. Kambe and P.D.Garn. Thermal Analysis, Kondansha Ltd. Toyo, 1974. 10. G.W. Ewing, Instrumental Methods, Of Analysis, 4th Ed. McFraw Hill Ltd., 1970. 11. N.H. Ring, Inorganic Polymers, Academic Press, New York, 1978 12. H.G. Heal, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorous, Academic Press, New York, 1980. 13. G.T. Seaborg, Man-made Transuranic Elements Preitce- Hall, 1963. 14. M.T.R. Series, The Superheavy Elements. 15. Haissilsky, Nuclear Chemistry and its Application, 1962. 16. S. Glasstone, Sourcebook of Aomic Energy, East-West Publisher, 1969. 17. D.Harvey, Modern Analytical Chemistry, The McGraw-Hill Pub, 1st Edition(2000); 18. John H. Block, E.B. Roche, T.P. Soine and Charles O. Wilson, Inorganic Medicinal and Pharmaceutical Chemistry, Lea and Febiger, 1974. 19. R. S. Drago, Physical Methods in Inorganic Chemistry, John-Wiley Pub., 1975 20. . M. Drescher an G. Jeschke, (Eds), EPR Spetroscopy: Applications in Chemistry and Biology, Springer-Verlag Berlin, Heidelberg 2012 21. Graham Smith; David Keeble. Introduction to Modern EPR Spectroscopy CRC Press 2013. 22. C.N.R. Rao, Chemical Applications of Infrared Spectroscopy Academic Pess, N.Y. (1963) 23. K. Veera Reddy, Symmetry and Spectroscopy, 24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell ; edition (2007) 25. . Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E., Horwood, (1990)
		<p>4. Applied Chemistry (Elective)</p> <p>4.1 Safety in Chemistry Laboratories (15 Lectures)</p> <p>4.1.1 Handling of Hazardous Materials</p> <p>4.1.2 Toxic Materials (Various types of toxins and their effects on humans)</p>

PSCHI EC-I 304	I	4.1.3 Explosives and Inflammable Materials 4.1.4 Types of fire extinguishers(chemical reaction) 4.1.5 Bioactive materials. 4.1.6 Recycling& recovery of metals with reference to Silver, lead, cobalt, Nickel and chromium 4.1.7 Laboratory Wastes Disposal Management in Chemical Laboratories .
	II	4.2 Manufacture and Applications of Inorganic Compounds-I(15Lectures) 4.2.1 Lime, Chlorine and Caustic soda, 4.2.2 Ceramics and refractory materials 4.2.3 Cement 4.2.4 Inorganic explosives (mercury fulminate, Lead azide)
	III	4.3 Manufacture and Applications of Inorganic Compounds-II (15 Lectures) 4.3.1 Fertilizers and micronutrients 4.3.2 Glass 4.3.3 Paints and Pigments
	IV	4.4 Metallurgy (15 Lectures) 4.4.1 Occurrence, extraction and metallurgy of Zirconium, Hafnium, Niobium, Tantalum Platinum and Palladium metals. 4.4.2 Physical and chemical properties and applications of these metals, 4.4.3 Compounds of these metals, alloys and their uses.
		<u>REFERENCES:</u> <ol style="list-style-type: none"> 1. G.M.Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995. 2. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007. 3. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic Pharmaceutical Chemistry, Nirali Prakashan, Pune, 19 . 4. D. A. Skoog, D. M. West, and F. J. Holler, Fundamentals of Analytical Chemistry, 7 th Edition, (printed in India in 2001), ISBN Publication. 5. B. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983.
	I	4.1 Inorganic Materials (15 Lectures) Elective (a) Classification, manufacture and applications of (i) Inorganic fibers, and (ii) Inorganic fillers. Study of (i) Condensed phosphates, and (ii) Coordination polymers. (b) Preparation, properties and uses of industrially important chemicals – potassium permanganate, sodium thiosulphate, bleaching powder, hydrogen peroxide, potassium

PSCHI EC-II 304		dichromate
	II	<p>4.2 Nuclear Chemistry and Inorganic Pharmaceuticals (15 Lectures)</p> <p>(a) Nuclear Chemistry : Introduction to of nuclear fuels and separation of fission products from spent fuel rods by PUREX process. Super heavy element, discovery, preparation, position in the periodic table.</p> <p>(b) Inorganic Pharmaceuticals : Radiopharmaceuticals containing Tc and Bi, contrast agents for X-ray and NMR imaging. Gastrointestinal agents viz. (i) antacids(aluminium hydroxide, milk of magnesia, sodium bicarbonate and (ii) Cathartics(magnesium sulphate and sodium phosphate). Topical agents viz.(i) protectives and adsorbents(talc, calamine), (ii) antimicrobial agents(potassium permanganate, tincture iodine, boric acid) and astringents(potash alum) .</p>
	III	<p>4.3 Advances in Nanomaterials: (15 Lectures)</p> <p>(a) Types of nanomaterials, e.g. nanotubes, nanorods, solid spheres, core-shell Inanoparticles, mesoporous materials; isolation of nano materials</p> <p>(b) Some important properties of nanomaterials: optical properties of metal and semiconductor nanoparticles, magnetic properties.</p> <p>(c) Some special nanomaterials: Carbon nanotubes: Types, synthesis using various methods, growth mechanism, electronic structure; Porous silicon: Preparation and mechanism of porous silicon formation, Factors affecting porous structure, properties of porous silicon; Aerogels: Types of aerogels, Properties and applications of aerogels.</p> <p>(d) Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental effects of nanotechnology</p>
	IV	<p>4.4 Some Selected Topics (15 Lectures)</p> <p>i) Isopoly and Hetropoly acids, ii) Supramolecular chemistry iii) Inorganic pesticides, and iv) Intercalation compounds</p>
		<p style="text-align: center;"><u>REFERENCES:</u></p> <ol style="list-style-type: none"> 1. G.M.Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995. 2. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007. 3. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic

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| | | <p>Pharmaceutical Chemistry, Nirali Prakashan, Pune, 19 .</p> <ol style="list-style-type: none"> 4. D. A. Skoog, D. M. West, and F. J. Holler, Fundamentals of Analytical Chemistry, 7 th Edition, (printed in India in 2001), ISBN Publication. 5. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983. |
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**PRACTICALS
SEMESTER-III**

PSCHI3P1: Analysis of ores/alloys

1. Analysis of Brass alloy:
 - (i) Cu content by iodometric method,
 - (ii) Zn content by complexometric method.
2. Analysis of Mangelium alloy:
 - (i) Al content by gravimetric method as basic succinate,
 - (ii) Mg content by complexometric method.
3. Analysis of Bronze alloy:
 - (i) Cu content by complexometric method,
 - (ii) Sn content by gravimetric method.
4. Analysis of steel nickel alloy:
 - (i) Ni content by homogeneous precipitation method.

PSCHI3P2: Solvent Extraction

1. Separation of Mn and Fe using isoamyl alcohol and estimation of Mn
2. Separation of Co and Ni using n-butyl alcohol and estimation of Co
3. Separation of U and Fe using 8-hydroxyquinoline in chloroform and estimation of U
4. Separation of Fe and Mo using isoamyl alcohol and estimation of Mo
5. Separation of Cu and Fe using n-butyl acetate and estimation of Cu

PSCHI3P3: Inorganic Preparations

1. Preparation of V(oxinate)₃
2. Preparation of Sn(IV) Iodide
3. Preparation of Co(α -nitroso- β -naphthol)₃
4. Preparation of Ni(salicylaldoxime)₂
5. Hexamine cobalt (III) chloride
6. Preparation of Trans-bis (glycinato) Cu(II)

PSCHI3P4: Analysis of the following samples

1. Calcium tablet for its calcium content by complexometric titration.
2. Bleaching powder for its available chlorine content by iodometric method.
3. Iron tablet for its iron content colorimetry by 1,10-phenonthroline method.
4. Calcium tablet for its calcium content by complexometric titration.
5. Bleaching powder for its available chlorine content by iodometric method.
6. Iron tablet for its iron content colorimetry by 1,10-phenonthroline method.

7. Nycil powder for its Zn content complexometrically.

Reference books for practicals

1. A. I. Vogel, *Quantitative Inorganic Analysis*.
2. J. D. Woolins, *Inorganic Experiments*.
3. Palmer, *Inorganic Preparations*.
4. G. Raj, *Advanced Practical Inorganic Chemistry*.
5. J. E. House, *Inorganic chemistry*, Academic press, 2nd edition, (2013).

SEMESTER IV		
Course Code	Unit	Topics
		(Numericals and word problems wherever possible.)
PSCHI 401	I	<p>1 Properties of Inorganic Solids and Group Theory.</p> <p>1.1 Electrical Properties- (15 Lectures)</p> <p>(a) Electrical properties of solids: (i) Conductivity: Solid Electrolytes; Fast Ion Conductors; Mechanism of Conductivity; Hopping Conduction.</p> <p>(b) Other Electrical Properties: Thomson and Seebeck Effects; Thermocouples and their Applications; Hall Effect; Dielectric, Ferroelectric, Piezoelectric and Pyroelectric Materials and their Inter-relationships and Applications</p>
	II	<p>1.2 Magnetic Properties. (15 Lectures)</p> <p>(a) Behaviour of substances in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering , superexchange, Hysteresis, Hard and soft magnets, structures and magnetic Properties of Metals and Alloys; Transition metal Oxides; Spinels; garnets, Ilmenites; Perovskite and Magneto plumbites, Application in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets.</p>
	III	<p>1.3 Thermal and Optical Properties (15 Lectures)</p> <p>a) Thermal Properties: Introduction, Heat Capacity and its Temperature Dependence; Thermal Expansion of Metals; Ceramics and Polymers and Thermal Stresses.</p> <p>(b) Optical properties: Color Centres and Birefringence; Luminescent and Phosphor Materials; Coordinate Model; Phosphor Model; Anti Stokes Phosphor; Ruby Laser; Neodymium Laser</p>
		1.4 Applications of group theory to –Electronic structures (15

	IV	<p>Lectures)</p> <p>(a) Recapitulation of Point groups and Character tables.</p> <p>(b) Transformation Properties of Atomic Orbitals;</p> <p>(c) Sigma and pi- molecular orbitals for AB₄ (tetrahedral) and AB₆ (octahedral) molecules;</p> <p>(d) Ligand Field Theory : Electronic structures of free atoms and ions; Splitting of levels and terms in a chemical environment; Construction of energy level diagrams; Direct product ; Correlation diagrams for d² ions in octahedral and tetrahedral ligand field; Methods of Ascending and Descending Symmetry; Hole formalism.</p>
		<p style="text-align: center;"><u>REFERENCE BOOKS</u></p> <ol style="list-style-type: none"> 1. L. E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005. 2. A.R. West, Solid State Chemistry and Its Applications, John Wiley & sons, 1987. 3. C.N.R. Rao and J.Gopalkrishnan New Directions in Solid State Chemistry, 2nd Ed., Cambridge University Press. 1997 4. L.V. Azaroff, Introduction to solids, Tata-McGraw Hill Book Co. New Delhi, 1977. 5. D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed. Wiley and sons, New York, 1966. 6. J.M. Hollas, Symmetry in Molecules, Chapman and Hall Ltd., 1972. 7. Reboert L carter, Molecular Symmetry and Group Hohn Wiley and Sons, New York, 1988. 8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993. 9. R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.. 10. H.V.Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993. Gary L.Miessler and Donald A.Tarr, Inorganic Chemistry, 3rd edition , Pearson Education, Inc., 2004. 11. D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996. 12. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press,N.Y. (1966)
	I	<p>2 Organometallics and main group Chemistry (15 Lectures)</p> <p>2.1 Organometallic Chemistry</p> <p>(a) Metal-Metal Bonding and Metal Clusters,</p> <p>(b) Electron Count and Structures of Clusters,,</p> <p>(c) Isolobal Analogy.</p> <p>(d)Organo Palladium and Organo Platinum Complexes (preparations, properties and applications.)</p> <hr/> <p>2.2 Applications of Organometallic Compounds (15 Lectures)</p>

PSCHI 402	II	(a) Catalysis-Homogenous and Heterogenous Catalysis: Comparison, Fundamental Reaction Steps. (b) Organometallics as Catalysts in Organic Reactions: (i)Hydrosilation, (ii)Hydroborationn. (iii)_Water gas Shifts Reaction (iv) Wacker process(Oxidation of alkenes) (v)Alcohol corbonylation (c)Coupling reactions : (i) Heck's reaction (ii) Suzuki reaction
	III	2.3 Inorganic cluster and cage compounds (15 Lectures) (i) Introduction, (ii) Bonding in boranes, (iii) Heteroboranes, (iv) Carboranes, (v) cluster compounds, (vi) electron precise compounds and their relation to clusters.
	IV	2.4 Inorganic ring and chain compounds (15 Lectures) (a) Silicates, polysilicates and aluminosilicates, (b) Phosphazenes, phosphazene polymers (c) Polyanionic and polycationic compounds
		<u>REFERENCES:</u>
		<ol style="list-style-type: none"> 1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., New Delhi; 2002. 2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3rd edition. 3. James E.Huheey, Inorganic Chemistry, 3rd edition, Harper & Row,Publishers, Asia, Pte Ltd., 1983. 4. W.W.Porterfield,Inorganic Chemistry-An Unified Approach,Academic press(1993); 5. D.F.Shriver, P.W.Atkins and C.H. Langford, Inorganic Chemistry,3rd edition Oxford University Press, 1999. 6. Asim K.Das, Fundamental Concepts of Inorganic Chemistry,(Volumes-I,II and III)CBS Pub.(2000) 7. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, Pergamon, 1984. 8. J.M.Hollas, Symmetry in Chemistry, Chapmanad Hall Ltd., NY, 1972.\ 9. F.A.Cotton, Chemical Applications of Group Theory, 2nd edition, Wiley Eastern Ltd., New Delhi , 1976 10. C.J.Ballhausen and H.B.Gray, Molecular Orbital Theory, MCGraw-Hill, New York, 1965. 11. H. Sisler, Chemistry in Non-aqueous Solvents: New York Reinhold Publ. 1965. 12. . J.J. Lagowski, The Chemistry of Non-aqueous Solvents, Academic press, New york and London. 13. . C.M. Day and Joel Selbin, Theoretical Inorganic Chemistry,Affiliated East West Press Pvt.Ltd., 1985. 14. L.E.Orgel, An Introduction to Ligand Field Theory , Methuen &

		<p>Co.Ltd., London, 1960.</p> <p>15. F.Basolo and R.G.Pearson, Mechanisms of Inorganic Reactions, Wiley, New York, 1967.</p> <p>16. . J.D.Lee, Concise Inorganic Chemistry, 5th ed., Blackwell ScienceLtd., 2005.</p> <p>17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New york, 1988.</p> <p>18. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2nd edition, John Wiley & sons, Inc., New York, 1992.</p> <p>19. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry, Prentice-Hall, (1997).</p> <p>20. . R.C.Mehrotra and A.Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt.Ltd., 2000.</p> <p>21. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983.</p> <p>22. James E.Huheey, Inoganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972).</p> <p>23. . F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.</p> <p>24. F.A. Cotton and R.A.Walton, Multiple Bonds between Metal Atoms, 2nd edition, claranden Press, Oxford, 1993.</p> <p>25. P.L. Soni, Vandana Soni ,Ane Books Pvt.,Ltd</p>
PSCHI 403	I	<p>3 Instrumental methods in Inorganic Chemistry .</p> <p>3.1 Spectroscopy (15 Lectures)</p> <p>(a) Infrared spectroscopy: Fundamental modes of vibrations, selection rules, IR absorption bands of metal - donor atom, effect of complexation on the IR spectrum of ligands formations on the IR of ligands like NH₃, CN⁻, CO, olefins (C=C) and C₂O₄²⁻ .</p> <p>(b) Raman spectroscopy: Raman spectroscopy for diatomic molecules. Determination of molecular structures like diatomic and triatomic molecules.</p>
		<p>(c) Applications of Group theory in Infrared and Raman spectroscopy.</p> <p>(c) Molecular Vibrations: Introduction; The Symmetry of Normal Vibrations; Determining the Symmetry Types of the Normal Modes; symmetry based Selection Rules of IR and Raman; Interpretation of IR and Raman Spectra for molecules such as H₂O, BF₃, N₂F₂, NH₃ and CH₄.</p>
		<p>(d) Nuclear Magnetic Resonance Spectroscopy :</p> <p>Introduction to basic principles and instrumentation. Use of ¹H, ¹⁹F, ³¹P, ¹¹B NMR spectra in structural elucidation of inorganic compounds; Spectra of paramagnetic materials: Contact shift, application of contact shift, lanthanide shift reagent.</p>
	II	<p>3.2 Microscopy of Surface Chemistry-I (15 Lectures)</p> <p>Introduction to surface spectroscopy, Microscopy, problems of surface analysis, distinction of surface species, sputter etching and depth profile and chemical imaging, instrumentations, Ion Scattering Spectra (ISS), Secondary Ion Mass Spectroscopy (SIMS), Auger Emission Spectroscopy</p>

		(AES),
	III	3.3 Microscopy of Surface Chemistry-II (15 Lectures) ESCA, Scanning Electron Microscopy (SEM), Atomic force microscopy (AFM) and transmission electron microscopy (TEM): Instrumentation and applications.
	IV	3.4 Thermal Methods (15 Lectures) 3.4.1 Application of TGA in Thermal characterization of polymers, quantitative analysis of mixture of oxalates, moisture content in coal, study of oxidation state of alloys etc. 3.4.2 Application of DSC and DTA in determination of thermodynamic parameters such as heat capacity and standard enthalpy of formation of the compounds, investigation of phase transitions, thermal stability of polymeric materials, purity of pharmaceuticals samples, M.P. and B.P. of organic compounds etc. 3.4.3 Basic principle, instrumentation and applications to other thermal methods like Thermomechanical analysis (TMA) and evolved gas analysis (EGA).
		<u>REFERENCES:</u>
		<ol style="list-style-type: none"> 1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis Fifth edition, (1996), ELBS Publication. Chapter 2, 3, 11. 2. W.H. Zachariasen. Theory of X-Ray Diffraction in Crystals. John Wiley. New York. 1946. 3. B.D. Cality,, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954. 4. R. Reaching, Electron Diffraction, Methuen and Co. London. 1936 5. May and Leopold, An Introduction to Mossbauer Spectroscopy, Plenum, New York, 1971. 6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, C.B.S. Publishers and Distributors, New Delhi, 1986. 7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press, Oxford, 1995. 8. Reverts John D., Nuclear Magnetic Resonance, McGraw Hill, New York, 1959. 9. . H. Kambe and P.D.Garn. Thermal Analysis, Kondansha Ltd. Toyo, 1974. 10. G.W. Ewing, Instrumental Methods, Of Analysis, 4th Ed. McFraw Hill Ltd., 1970. 11. N.H. Ring, Inorganic Polymers, Academic Press, New York, 1978 12. H.G. Heal, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorous, Academic Press, New York, 1980. 13. G.T. Seaborg, Man-made Transuranic Elements Preitce- Hall, 1963. 14. M.T.R. Series, The Superheavy Elements.

		<p>15. Haissilsky, Nuclear Chemistry and its Application, 1962.</p> <p>16. S. Glasstone, Sourcebook of Atomic Energy, East-West Publisher, 1969.</p> <p>17. D. Harvey, Modern Analytical Chemistry, The McGraw-Hill Pub, 1st Edition (2000);</p> <p>18. John H. Block, E.B. Roche, T.P. Soine and Charles O. Wilson, Inorganic Medicinal and Pharmaceutical Chemistry, Lea and Febiger, 1974.</p> <p>19. R. S. Drago, Physical Methods in Inorganic Chemistry, John-Wiley Pub., 1975</p> <p>20. . M. Drescher and G. Jeschke, (Eds), EPR Spectroscopy: Applications in Chemistry and Biology, Springer-Verlag Berlin, Heidelberg 2012</p> <p>21. Graham Smith; David Keeble. Introduction to Modern EPR Spectroscopy CRC Press 2013.</p> <p>22. C.N.R. Rao, Chemical Applications of Infrared Spectroscopy Academic Press, N.Y. (1963)</p> <p>23. K. Veera Reddy, Symmetry and Spectroscopy,</p> <p>24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell ; edition (2007)</p> <p>25. . Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E., Horwood, (1990)</p>
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Course Code: PSCHIOC-I 404
Paper – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1:	[15L]
Introduction to Intellectual Property:	[2L]
[2L]	
Historical Perspective, Different types of IP, Importance of protecting IP.	
Patents:	[5L]
[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]
[2L]	
Definition, How to obtain, features, International design registration.	
Copyrights:	[2L]

[2L]

Introduction, How to obtain, Differences from Patents.

Trade Marks:

[2L]

[2L]

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications:

[2L]

[2L]

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

Unit 2:

[15L]

[15L]

Trade Secrets:

[2L]

[2L]

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

IP Infringement issue and enforcement:

[2L]

[2L]

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

Economic Value of Intellectual Property:

[2L]

[5L]

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

Different International agreements:

[6L]

(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]

[15L]

Introduction to Cheminformatics:

[5L]

[5L]

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

Representation of molecules and chemical reactions:

[5L]

[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]

[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]

[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.

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PAPER – IV: RESEARCH METHODOLOGY

Unit 1:

[15L]

Print:

[5L]

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, textbooks, 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 SCIENTIFIC PAPERS

[15L]

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 Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

PRACTICALS SEMESTER-IV

PSCHI4P1: Analysis of Ores

1. Analysis of galena ore:
 - (i) Pb content as PbCrO₄ by gravimetric method using 5% potassium chromate,
 - (ii) Fe content by colorimetrically using 1, 10- phenonthroline.
2. Analysis of Zinc blend ore:
 - (i) Zn content by complexometric method,
 - (ii) Fe content by colorimetric method (Azide method).
3. Analysis of Pyrolusite ore:
 - (i) Mn content by complexometric method,
 - (ii) Acid insoluble residue by gravimetric method.

PSCHI4P2: Coordination Chemistry

1. Determiation of Stability constant of $[\text{Zn}(\text{NH}_3)_4]^{2+}$ by potentiometry
2. Determiation of Stability constant of $[\text{Ag}(\text{en})]^+$ by potentiometry
3. Determiation of Stability constant of $[\text{Fe}(\text{SCN})]^{2+}$ by slope ratio method
4. Determiation of CFSE values of hexa-aqua complexes of Ti^{3+} and Cr^{3+} .
5. Determiation of Racah parameters for complex $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ and $[\text{Ni}(\text{en})_3]^{2+}$

PSCHI4P3: Analysis of the following samples

1. Electral powder for Na/K content flame photometrically.
2. Fasting salt for chloride content conductometrically.
3. Sea water for percentage salinity by Volhard's method.
4. Soil for mixed oxide content by gravimetric method.
5. Fertilizer for potassium content by flame photometry.

PSCHI4P4: Project Evaluation & Spectral interpretation

Reference books for practicals	
1.	A. I. Vogel, <i>Quantitative Inorganic Analysis</i> .
2.	J. D. Woolins, <i>Inorganic Experiments</i> .
3.	Palmer, <i>Inorganic Preparations</i> .
4.	G. Raj, <i>Advanced Practical Inorganic Chemistry</i> .
5.	J. E. House, <i>Inorganic chemistry</i> , Academic press, 2 nd edition, (2013).